

L Number	Hits	Search Text	DB	Time stamp
11	39	azulen	USPAT; US-PGPUB	2002/05/15 21:20
12	0	cyclopenta with azulene	USPAT; US-PGPUB	2002/05/15 21:19

9/995,324

09/ 995,324

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TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web  
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NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency  
NEWS 5 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02  
NEWS 6 Mar 08 Gene Names now available in BIOSIS  
NEWS 7 Mar 22 TOXLIT no longer available  
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NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/Caplus and USPATFULL  
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NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 14 Apr 09 ZDB will be removed from STN  
NEWS 15 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUIDB  
NEWS 16 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 17 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 18 Apr 22 Federal Research in Progress (FEDRIP) now available  
  
NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002  
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

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09/ 995,324

FILE 'REGISTRY' ENTERED AT 14:47:41 ON 09 MAY 2002  
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TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

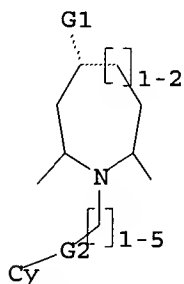
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES  
for more information. See STNote 27, Searching Properties in the CAS  
Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 09995324.str

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



G1 H,O  
G2 O,S,N,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 14:48:01 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 20299 TO ITERATE

4.9% PROCESSED 1000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 397477 TO 414483  
PROJECTED ANSWERS: 135 TO 675

L2 1 SEA SSS SAM L1

=> s l1 ful

09/ 995,324

FULL SEARCH INITIATED 14:48:09 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 405697 TO ITERATE

98.6% PROCESSED 400000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.16

285 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 405697 TO 405697  
PROJECTED ANSWERS: 285 TO 340

L3 285 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

140.66

140.87

FILE 'CAPLUS' ENTERED AT 14:48:37 ON 09 MAY 2002  
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FILE COVERS 1907 - 9 May 2002 VOL 136 ISS 19  
FILE LAST UPDATED: 7 May 2002 (20020507/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l3

L4 96 L3

=> s (cyclopent? and azulen?) and l4

101605 CYCLOPENT?

5027 AZULEN?

L5 0 (CYCLOPENT? AND AZULEN?) AND L4

=> s l4 and azulen?

5027 AZULEN?

L6 0 L4 AND AZULEN?

=> s l4 and (dithia and aza)

1794 DITHIA

13403 AZA

L7 0 L4 AND (DITHIA AND AZA)

09/ 995,324

=> d l4 1- ibib abs fhitr

YOU HAVE REQUESTED DATA FROM 96 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:59016 CAPLUS

DOCUMENT NUMBER: 136:257030

TITLE: Novel Tricyclic-.alpha.-alkoxyphenylpropionic Acids:  
Dual PPAR.alpha./.gamma. Agonists with Hypolipidemic  
and Antidiabetic Activity

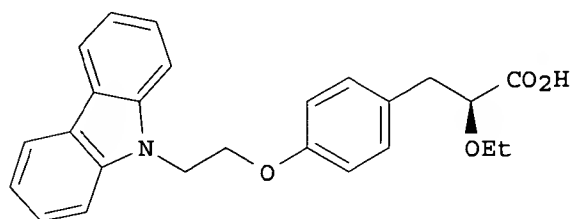
AUTHOR(S): Sauerberg, Per; Pettersson, Ingrid; Jeppesen, Lone;  
Bury, Paul S.; Mogensen, John P.; Wassermann, Karsten;  
Brand, Christian L.; Sturis, Jeppe; Woeldike, Helle  
F.; Fleckner, Jan; Andersen, Anne-Sofie T.; Mortensen,  
Steen B.; Svensson, L. Anders; Rasmussen, Hanne B.;  
Lehmann, Soren V.; Polivka, Zdenek; Sindelar, Karel;  
Panajotova, Vladimira; Ynddal, Lars; Wulff, Erik M.  
CORPORATE SOURCE: Novo Nordisk Park, Novo Nordisk A/S, Malov, 2760, Den.  
SOURCE: Journal of Medicinal Chemistry (2002), 45(4), 789-804  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



*late*

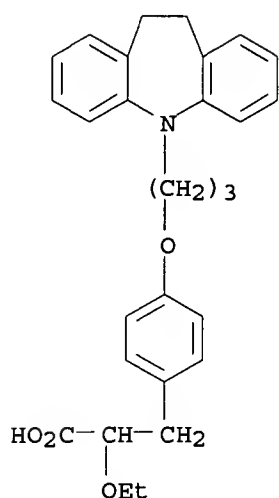
AB Tricyclic .alpha.-ethoxy phenylpropionic acid derivs. such as nonracemic carbazoleethoxypropionic acid I were prepd. and tested for their PPAR.alpha. and PPAR.gamma. agonist activities as potential antihyperlipidemic and antidiabetic agents. Mol. mechanics and X-ray crystallog. data of the complex of the PPAR.gamma. receptor with I were obtained. Db/db mice treated with I showed improved insulin sensitivity over treatment with either pioglitazone or rosiglitazone, suggesting in vivo PPAR.gamma. activity. Rats fed a high-cholesterol diet and treated with I also showed decreased plasma triglycerides and cholesterol after 4 days treatment, indicating in vivo PPAR.alpha. activity. Pharmacokinetics of selected compds. suggested that extended drug exposure improved the in vivo activity of in vitro active compds.

IT 265301-15-3P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and PPAR.alpha. and PPAR.gamma. agonist activity of tricyclic .alpha.-ethoxyphenylpropionic acids prepd. as potential antihyperlipidemic and antidiabetic agents)

RN 265301-15-3 CAPLUS

CN Benzenepropanoic acid, 4-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propoxy]-.alpha.-ethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:10247 CAPLUS

DOCUMENT NUMBER: 136:74317

TITLE: Cosmetic compositions containing iminodibenzyl or fluorene derivatives

INVENTOR(S): Bajor, John Steven; Pocalyko, David Joseph

PATENT ASSIGNEE(S): Unilever Plc, UK; Unilever Nv; Hindustan Lever Ltd.

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000186	A2	20020103	WO 2001-EP6373	20010605
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002028804	A1	20020307	US 2001-873159	20010601
US 6355687	B1	20020312		

PRIORITY APPLN. INFO.: US 2000-215648P P 20000630

AB Cosmetic methods and compns. contg. selected iminodibenzyl or fluorene derivs. are described. When used for skin or hair care, the compns. provide control of sebum secretion from sebocytes, improved oil control and improved feel, and prevent shine and stickiness. Thus, a iminodibenzyl deriv. (1 .mu.M) and retinol (1 .mu.M) in a cosmetic compn. showed sebum suppression activity.

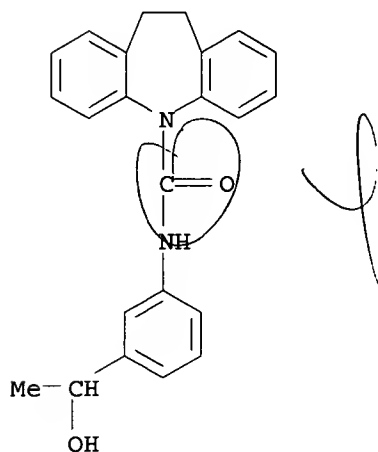
IT 384847-27-2

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(cosmetic compns. contg. iminodibenzyl or fluorene derivs.)

RN 384847-27-2 CAPLUS

09/ 995,324

CN 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:895650 CAPLUS

DOCUMENT NUMBER: 136:37404

TITLE: Preparation of phenyl amides and ureas as neuropeptide Y5 receptor antagonists

INVENTOR(S): Dugar, Sundeep; Neustadt, Bernard R.; Stamford, Andrew W.; Wu, Yusheng

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S., 42 pp.

CODEN: USXXAM

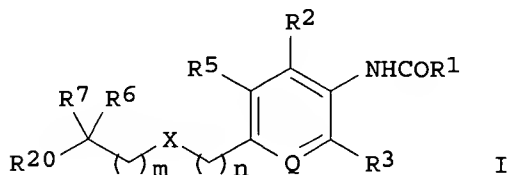
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6329395	B1	20011211	US 1999-326575	19990607
PRIORITY APPLN. INFO.:			US 1998-88422P	P 19980608
OTHER SOURCE(S):	MARPAT 136:37404			
GI				



AB The title compds. [I; m, n = 0-2, provided that the sum m + n = 0-3; Q = CR4, N; X = O, S, SO, etc.; R1 = (un)substituted aryl, heteroaryl, amino, etc.; R2-R5 = H, alkyl, (un)substituted cycloalkyl, etc.; R6, R7 = H, alkyl, alkenyl, etc.; CR6R7 = 3-7-membered carbocyclic ring, 4-7-membered heterocyclic ring; R20 = alkyl, cycloalkyl, hydroxyalkyl, etc.], useful in the treatment of eating disorders and diabetes, were prepd. Thus, amidation of 4-[1,1-dimethylbutylthio]aniline with trimethylacetyl chloride in CH2Cl2 afforded 76% I [Q = CH; R1 = Me3C; R2 = R3 = R5 = H; R6

= R7 = Me; R20 = Pr; X = S; m = n = 0] which showed Ki of 3 nM against human NPY5 receptor binding.

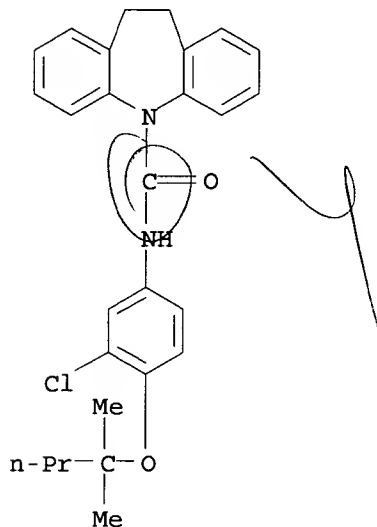
IT **252346-34-2P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of Ph amides and ureas as neuropeptide Y5 receptor antagonists)

RN 252346-34-2 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, N-[3-chloro-4-(1,1-dimethylbutoxy)phenyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:489367 CAPLUS

DOCUMENT NUMBER: 135:76874

TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C

INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan

SOURCE: PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

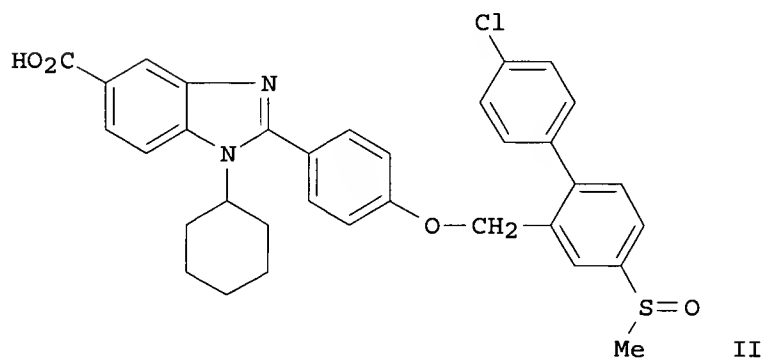
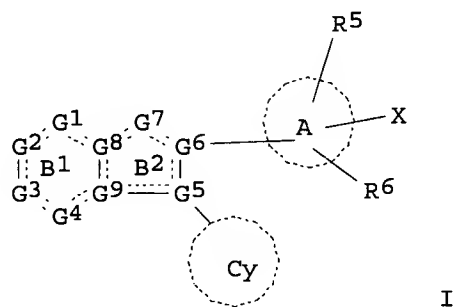
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			



09/ 995,324

EP 1162196            A1    20011212            EP 2000-987728    20001222  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO  
BR 2000008525        A    20020102            BR 2000-8525        20001222  
JP 2001247550        A2   20010911            JP 2000-391904      20001225  
NO 2001004134        A    20011022            NO 2001-4134        20010824  
PRIORITY APPLN. INFO.:            JP 1999-369008    A   19991227  
   WO 2000-JP9181    W   20001222  
OTHER SOURCE(S):            MARPAT 135:76874  
GI



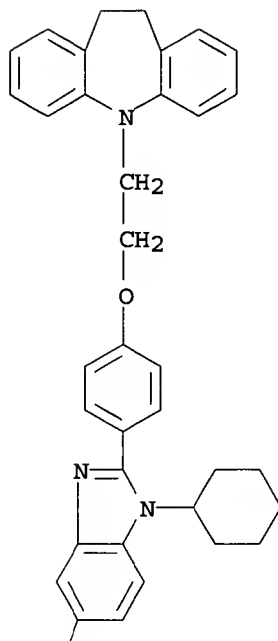
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2; G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 .mu.M against hepatitis C virus polymerase. A formulation is given.

IT **347166-36-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347166-36-3 CAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:756707 CAPLUS

DOCUMENT NUMBER: 133:321874

TITLE: Preparation of malonic acid derivatives useful in the treatment and/or prevention of conditions mediated by Peroxisome Proliferator-Activated Receptors

INVENTOR(S): Jeppesen, Lone; Sauerberg, Per; Murray, Anthony; Bury, Paul Stanley

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

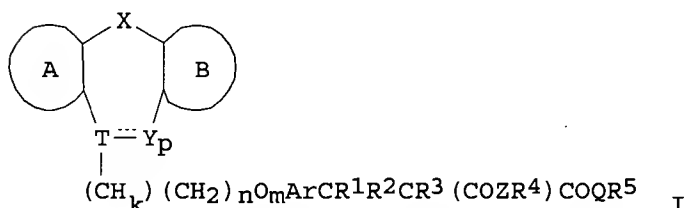
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000063209	A1	20001026	WO 2000-DK191	20000417

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,

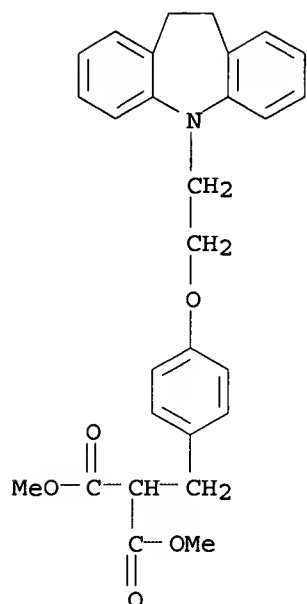
*Applicant's*

09/ 995,324

AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
EP 1171438 A1 20020116 EP 2000-918726 20000417  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO  
US 2002010171 A1 20020124 US 2001-878670 20010611  
PRIORITY APPLN. INFO.: DK 1999-535 A 19990420  
WO 2000-DK191 W 20000417  
US 2000-551497 A1 20000418  
OTHER SOURCE(S): MARPAT 133:321874  
GI



- AB The title compds. I [ring A and ring B, fused to the ring contg. X and T, independently of each other represents a 5-6 membered cyclic ring, optionally substituted; T is N or CR<sub>14</sub>; Y is C, O, S, CO, SO, SO<sub>2</sub>, NR<sub>11</sub>; k = 1, 2; Ar = arylene, heteroarylene, divalent heterocyclic group; R<sub>1</sub> = H, OH, halo, alkoxy, etc.; R<sub>2</sub> = H, OH, alkyl, alkynyl, etc.; R<sub>3</sub> = H, OH, alkyl, etc.; R<sub>4</sub> = H, alkenyl, aryl, etc.; R<sub>5</sub> = H, alkyl, heteroaryl, etc.; Z = O, NR<sub>12</sub>; Q = O, NR<sub>13</sub>; n = 0-3; m = 0-1; p = 0-1], useful in the treatment and/or prevention of conditions mediated by nuclear receptors, in particular the Peroxisome Proliferator-Activated Receptors (PPAR), were prepd. E.g., 2-[4-(2-.beta.-carbolin-9-yl-ethoxy)benzyl]malonic acid hydrochloride was prepd.
- IT 302589-16-8P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of malonic acid derivs. useful in the treatment and/or prevention of conditions mediated by peroxisome proliferator-activated receptors)
- RN 302589-16-8 CAPLUS
- CN Propanedioic acid, [[4-[2-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)ethoxy]phenyl]methyl]-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:403682 CAPLUS

DOCUMENT NUMBER: 133:222478

TITLE: A new diastereoselective approach to simplified dynemicin analogues

AUTHOR(S): Guanti, Giuseppe; Riva, Renata

CORPORATE SOURCE: Dip. Chim. Chim. Ind. and C.N.R., CSCCCA, Universita di Genova, Genoa, Italy

SOURCE: Chemical Communications (Cambridge) (2000), (13), 1171-1172

CODEN: CHCOFS; ISSN: 1359-7345

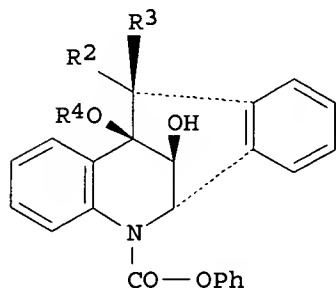
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:222478

GI



I

AB The stereoselective synthesis of new simplified dynemicin analogs (I) ( $R_2 = \text{Me}$ ,  $R_3 = \text{H}$ ,  $R_4 = \text{Ts}$ ;  $R_2 = R_4 = \text{H}$ ,  $R_3 = \text{Me}$ ) is reported: key steps of the sequence are the regio- and diastereoselective functionalization of a quinoline nucleus, bearing a substituent with a stereogenic center, and

the formation of the 10-membered cyclic enediyne system by Pd-catalyzed Stille-like reaction.

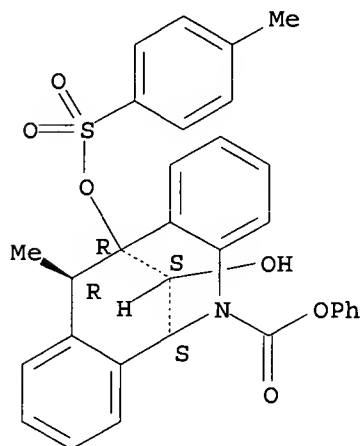
IT 291743-75-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(diastereoselective approach to simplified dynemicin analogs)

RN 291743-75-4 CAPLUS

CN 6,12-Methanodibenz[b,f]azocine-5(6H)-carboxylic acid, 11,12-dihydro-13-hydroxy-11-methyl-12-[[[4-methylphenyl)sulfonyl]oxy]-, phenyl ester, (6R,11S,12S,13R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:383927 CAPLUS

DOCUMENT NUMBER: 133:34425

TITLE: Pharmaceutical compositions containing N-substituted azaheterocyclic compounds for the treatment of indications related to angiogenesis

INVENTOR(S): Hansen, Anker Jon; Jorgensen, Tine Krogh; Olsen, Uffe Bang

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000032193	A1	20000608	WO 1999-DK671	19991201
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1135129	A1	20010926	EP 1999-957964	19991201
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

IE, SI, LT, LV, FI, RO  
 US 2002045610 A1 20020418  
 PRIORITY APPLN. INFO.:

US 2001-872127 20010601  
 DK 1998-1586 A 19981202  
 US 1998-111445P P 19981208  
 WO 1999-DK671 W 19991201

OTHER SOURCE(S): MARPAT 133:34425

AB The present invention relates to the use of N-substituted azaheterocyclic compds. or salts thereof, for the treatment of conditions related to angiogenesis. N-substituted azaheterocyclic compds. decreased the vessel area of neovascularization of mouse cornea by 30-50%. A tablet contained a N-substituted azaheterocyclic compd. 100, silicone dioxide 1.5, microcryst. cellulose 70, modified cellulose gum 7.5, in the core, and hydroxypropyl Me cellulose 9, and Mywacett 9-40T 0.9 mg in the coating.

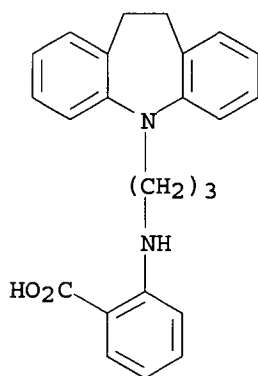
IT 183476-83-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmaceutical compns. contg. N-substituted azaheterocyclic compds. for treatment of indications related to angiogenesis)

RN 183476-83-7 CAPLUS

CN Benzoic acid, 2-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]amino]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:277964 CAPLUS

DOCUMENT NUMBER: 132:308362

TITLE: Preparation of tricyclic compounds for the treatment and/or prevention of conditions mediated by nuclear receptors, in particular the Peroxisome Proliferator-Activated Receptors (PPAR)

INVENTOR(S): Jeppesen, Lone; Bury, Paul Stanley; Sauerberg, Per  
 PATENT ASSIGNEE(S): Novo Nordisk A/s, Den.; Reddy's Research Foundation  
 SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000023425	A1	20000427	WO 1999-DK570	19991019
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,				

IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,  
 MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,  
 SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,  
 BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 AU 9961902 A1 20000508 AU 1999-61902 19991019  
 EP 1123279 A1 20010816 EP 1999-948738 19991019  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO  
 PRIORITY APPLN. INFO.: DK 1998-1352 A 19981021  
 WO 1999-DK570 W 19991019  
 OTHER SOURCE(S): MARPAT 132:308362  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

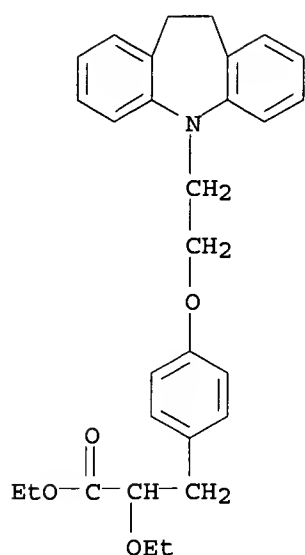
AB The title compds. [I; R1-R4 = H, halo, perhalomethyl, etc.; R1 and R2, R2 and R3, R3 and R4 may form (un)substituted cyclic ring contg. 5-7 carbon atoms; A = (un)substituted 5-6 membered cyclic ring; X = a bond, CH:CH, OCH2O, etc.; Ar = (un)substituted arylene, heteroarylene, divalent heterocyclic group; R5 = H, OH, halo, etc.; R6 = H, OH, halo, etc.; R7 = H, alkyl, alkenyl, etc.; R8 = H, alkyl, alkenyl, etc.; Y = O, S, NH, etc.; n = 1-4; m = 0-1], useful in the treatment and/or prevention of conditions mediated by nuclear receptors, in particular the Peroxisome Proliferator-Activated Receptors (PPAR) (e.g., in the treatment of diabetes and/or obesity), were prepd. and formulated. Thus, reacting 2-(10,11-dihydrodibenzo[b,f]azepin-5-yl)ethanol with Et 2-ethoxy-3-(4-hydroxyphenyl)propionate in the presence of triphenylphosphine and di-Et azodicarboxylate afforded 90% II. Compds. I are effective at 0.1-70 mg/day in the treatment of adult humans.

IT 265300-87-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (prepn. of tricyclic compds. for the treatment and/or prevention of conditions mediated by nuclear receptors, in particular the Peroxisome Proliferator-Activated Receptors (PPAR))

RN 265300-87-6 CAPLUS

CN Benzenepropanoic acid, 4-[2-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)ethoxy]-.alpha.-ethoxy-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:113097 CAPLUS

DOCUMENT NUMBER: 132:151671

TITLE: Preparation of indoline derivatives and 1,2,3,4-tetrahydroquinoline derivatives useful for the treatment or prophylaxis of neurological injury and neurodegenerative disorders

INVENTOR(S): Reddy, N. Laxma; Maillard, Michael; Berlove, David; Magar, Sharad; Durant, Graham J.

PATENT ASSIGNEE(S): Cambridge Neuroscience, Inc., USA

SOURCE: U.S., 41 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

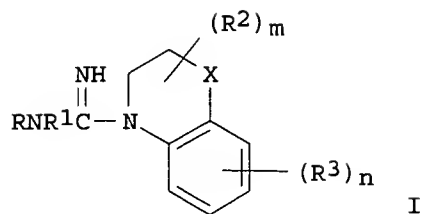
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6025355	A	20000215	US 1997-858399	19970519
US 6358993	B1	20020319	US 1999-425582	19991022
PRIORITY APPLN. INFO.:			US 1996-601992	B2 19960215
			WO 1997-US2678	A1 19970214
			US 1997-858399	A3 19970519

OTHER SOURCE(S): MARPAT 132:151671

GI





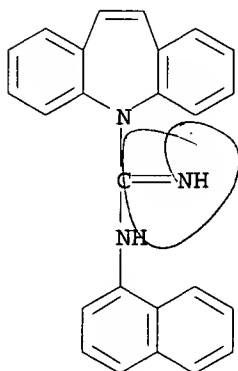
AB The title compds., e.g. I (R, R1 = H, alkyl, alkenyl, alkoxy, alkylthio, etc.; R2, R3 = H, halo, OH, alkyl, etc.; X = sulfinyl, sulfonyl; m, n = 0-4), useful for the treatment or prophylaxis of neurol. injury and neurodegenerative disorders, were prepd. E.g., N-(1-naphthyl)-4-(2,3-dihydro[1,4]benzothiazinyl)carboximidamide was prepd. Anticonvulsant activity of some of the compds. was detd.

IT 195437-37-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. and anticonvulsant activity of indoline derivs. and 1,2,3,4-tetrahydroquinoline derivs.)

RN 195437-37-7 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboximidamide, N-1-naphthalenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 198 THERE ARE 198 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:97545 CAPLUS

DOCUMENT NUMBER: 132:251016

TITLE: Synthesis and reactivity of novel fluorinated tricyclic dynemicin A mimic

AUTHOR(S): Kim, Jung Hee; Ryoo, Keon Sang; Choi, Jong-Ha; Hong, Yong Pyo

CORPORATE SOURCE: Department of Chemistry, Andong National University, Andong, 760-749, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2000), 21(1),

PUBLISHER:

Korean Chemical Society

DOCUMENT TYPE:

Journal

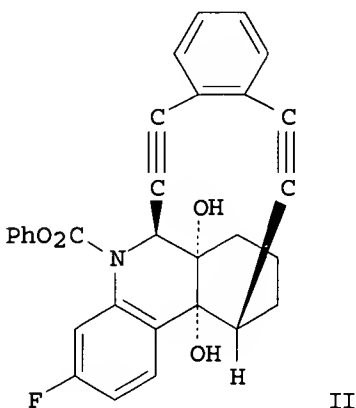
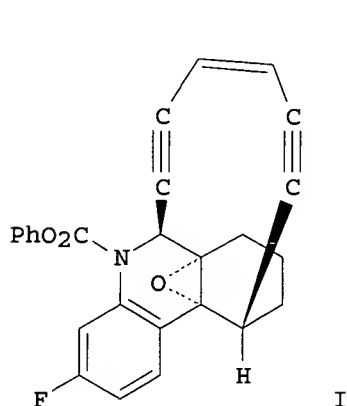
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 132:251016

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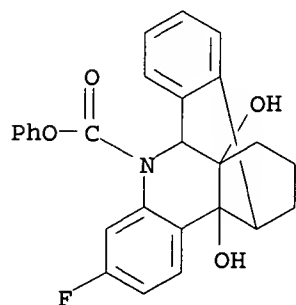
AB The authors describe the synthesis of a novel fluorinated tricyclic dynemicin A mimic (I) and its Bergman cycloaromatization to (II).

IT 263011-80-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis and reactivity of novel fluorinated tricyclic dynemicin A mimic)

RN 263011-80-9 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid, 3-fluoro-11,12-dihydro-12,13-dihydroxy-, phenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:52180 CAPLUS

DOCUMENT NUMBER: 132:190716

TITLE:

Structure-activity relationship and site of binding of polyamine derivatives at the nicotinic acetylcholine receptor

AUTHOR(S): Bixel, M. Gabriele; Krauss, Michael; Liu, Ying; Bolognesi, Maria L.; Rosini, Michela; Mellor, Ian S.; Usherwood, Peter N. R.; Melchiorre, Carlo; Nakanishi, Koji; Hucho, Ferdinand

CORPORATE SOURCE: Institut fur Biochemie, Freie Universitat Berlin, Berlin, D-14195, Germany

SOURCE: European Journal of Biochemistry (2000), 267(1), 110-120  
CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Blackwell Science Ltd.

DOCUMENT TYPE: Journal

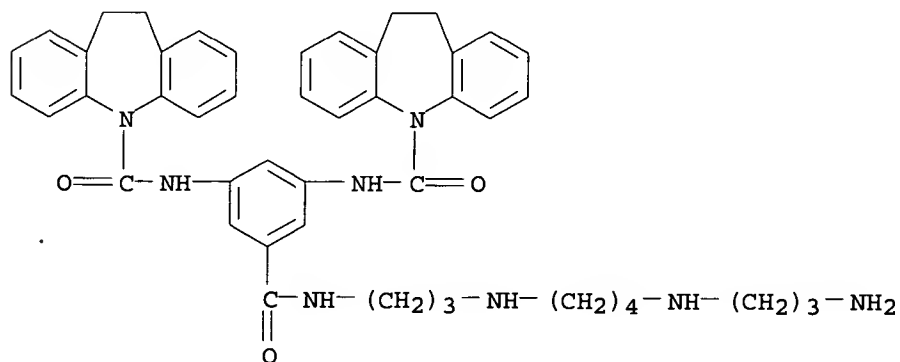
LANGUAGE: English

AB Several wasp venoms contain philanthotoxins (PhTXs), natural polyamine amides, which act as noncompetitive inhibitors (NCIs) on the nicotinic acetylcholine receptor (nAChR). Effects of varying the structure of PhTXs and poly(methylene tetramine)s on the binding affinity have been investigated. Using the fluorescent NCI ethidium in a displacement assay Kapp values of these compds. have been detd. We found that an increase in size of the PhTX's hydrophobic head group significantly increased the binding affinity, while inserting pos. charge almost completely destroyed it. Elongating the PhTX polyamine chain by introducing an addnl. aminomethylene group decreased the binding affinity, whereas a terminal lysine improved it. In general, poly(methylene tetramine)s showed higher binding affinities than PhTX analogs. The stoichiometry of PhTX binding was detd. to be two PhTX mols. per receptor monomer. PhTXs appeared to bind to a single class of nonallosterically interacting binding sites and bound PhTX was found to be completely displaced by well-characterized luminal NCIs. To elucidate the site of PhTX binding, a photolabile, radioactive PhTX deriv. was photocrosslinked to the nAChR in its closed channel conformation resulting in labeling yields for the two .alpha. and the .beta., .gamma. and .delta. subunits of 10.4, 11.1, 4.0 and 7.4%, resp. Based on these findings we suggest that PhTXs and poly(methylene tetramine)s enter the receptor's ionic channel from the extracellular side. The hydrophobic head groups most likely bind to the high-affinity NCI site, while the pos. charged polyamine chains presumably interact with the neg. charged selectivity filter located deep in the channel lumen.

IT 175085-76-4  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(structure-activity relationship and site of binding of polyamine derivs. at nicotinic acetylcholine receptor)

RN 175085-76-4 CAPLUS

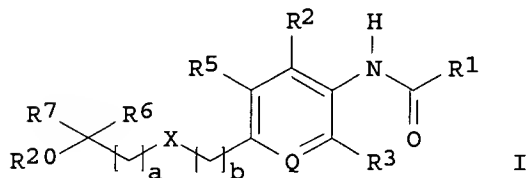
CN 5H-Dibenz[b,f]azepine-5-carboxamide, N,N'-[5-[[[3-[[4-[(3-aminopropyl)amino]butyl]amino]propyl]amino]carbonyl]-1,3-phenylene]bis[10,11-dihydro- (9CI) (CA INDEX NAME)



RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1999:795789 CAPLUS  
 DOCUMENT NUMBER: 132:35516  
 TITLE: Preparation of phenyl amides and ureas as neuropeptide Y5 receptor antagonists  
 INVENTOR(S): Dugar, Sundeep; Neustadt, Bernard R.; Stamford, Andrew W.; Wu, Yusheng  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: PCT Int. Appl., 67 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964394	A1	19991216	WO 1999-US11795	19990607
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MD, MG, MK, MN, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9943178	A1	19991230	AU 1999-43178	19990607
EP 1086078	A1	20010328	EP 1999-955470	19990607
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
PRIORITY APPLN. INFO.:			US 1998-93132	A2 19980608
			WO 1999-US11795	W 19990607
OTHER SOURCE(S):			MARPAT 132:35516	
GI				



AB The title compds. [I; a, b = 0-2, provided that the sum a + b = 0-3; Q = CR4, N; X = O, S, SO, etc.; R1 = (un)substituted aryl, heteroaryl, amino, etc.; R2-R5 = H, alkyl, (un)substituted cycloalkyl, etc.; R6, R7 = H, alkyl, alkenyl, etc.; CR6R7 = 3-7-membered carbocyclic ring, 4-7-membered heterocyclic ring; R20 = alkyl, cycloalkyl, hydroxyalkyl, etc.], useful in the treatment of eating disorders and diabetes, were prepd. Thus, amidation of 4-[4,4-dimethylbutylthio]aniline with trimethylacetyl chloride in CH2Cl2 afforded 76% I [Q = CH; R1 = Me3C; R2 = R3 = R5 = H; R6 = R7 = Me; R20 = Pr; X = S; a = b = 0]. For the compds. I, a range of neuropeptide Y5 receptor binding activity from 0.1-1000 nM was obsd.

IT 252346-34-2P

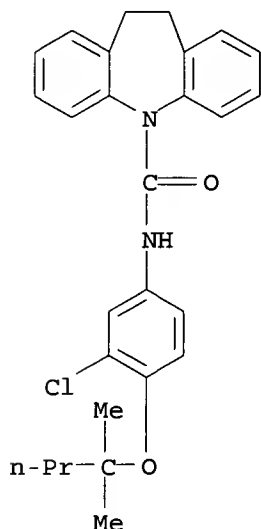
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of Ph amides and ureas as neuropeptide Y5 receptor antagonists)

RN 252346-34-2 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, N-[3-chloro-4-(1,1-dimethylbutoxy)phenyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:512075 CAPLUS

DOCUMENT NUMBER: 131:286423

TITLE: One-pot synthesis of pharmacologically active diamines via rhodium-catalyzed carbonylative hydroaminomethylation of heterocyclic allylic amines

AUTHOR(S): Rische, Thorsten; Muller, Kai-Sven; Eilbracht, Peter  
CORPORATE SOURCE: Organische Chemie I (FB 3), Universitat Dortmund, Dortmund, D-44221, Germany

SOURCE: Tetrahedron (1999), 55(32), 9801-9816

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:286423

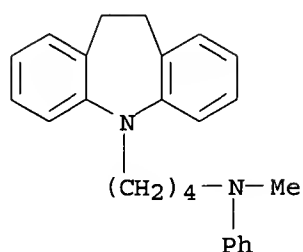
AB Pharmacol. active derivs. of phenothiazine, iminodibenzyl, carbazole and pyrazole are prepd. with high yields and chemoselectivity by the reaction of the corresponding N-allylic or N-methallylic compds., primary or secondary amines, carbon monoxide and hydrogen in the presence of [Rh(cod)Cl]<sub>2</sub> as catalyst via a one pot hydroformylation-amine condensation-redn. sequence.

IT 246041-29-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(one-pot synthesis of diamines via rhodium-catalyzed carbonylative hydroaminomethylation of heterocyclic allylic amines)

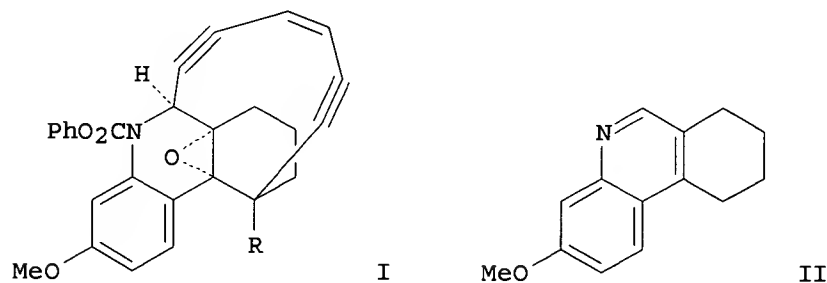
RN 246041-29-2 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-butanamine, 10,11-dihydro-N-methyl-N-phenyl- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1998:750949 CAPLUS  
 DOCUMENT NUMBER: 130:95404  
 TITLE: Epoxide opening and Bergman cyclization of tricyclic enediyne models possessing a methoxy group  
 AUTHOR(S): Hong, Yong Pyo; Kwon, Soon Ho  
 CORPORATE SOURCE: Department of Chemistry, Andong National University, Andong, 760-749, S. Korea  
 SOURCE: Bulletin of the Korean Chemical Society (1998), 19(11), 1150-1151  
 CODEN: BKCSDE; ISSN: 0253-2964  
 PUBLISHER: Korean Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 130:95404  
 GI



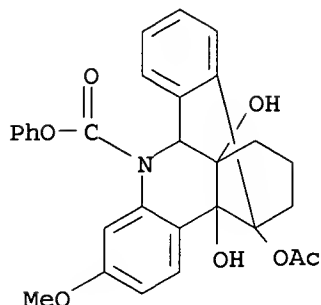
AB The introduction of a methoxy group at C3 of tricyclic dynemicin A model compds. activated the epoxide opening and Bergman cyclization under acidic conditions. Thus the enediyne target compd. I (R = OAc) was prepd. from II via the cyclized I (R = OH) to protect pinacol-pinacolone rearrangement under Bergman cyclization conditions. The acid-induced epoxide opening followed by Bergman cyclization of I (R = OAc) was performed with p-toluenesulfonic acid in benzene/1,4-cyclohexadiene at 40.degree..

IT 219509-95-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of tricyclic enediyne dynemicin A model compds. possessing a methoxy group at C3 that activate epoxide opening and Bergman cyclization under acidic conditions)

RN 219509-95-2 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid, 11-(acetyloxy)-11,12-dihydro-12,13-dihydroxy-3-methoxy-, phenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:727783 CAPLUS

DOCUMENT NUMBER: 130:90087

TITLE: Serine proteases-directed small molecule probe libraries

AUTHOR(S): Dhanoa, Dale S.; Soll, Richard M.; Subasinghe, Nalin; Wu, Zhengdong; Rinker, James; Hoffman, James; Eisennagel, Stephen; Graybill, Todd; Bone, Roger; Radzicka, Anna; Murphy, Larry; Salemm, F. Raymond

CORPORATE SOURCE: 3-Dimensional Pharmaceuticals, Inc., Exton, PA, 19341, USA

SOURCE: Medicinal Chemistry Research (1998), 8(4/5), 187-205  
CODEN: MCREEB; ISSN: 1054-2523

PUBLISHER: Birkhaeuser Boston

DOCUMENT TYPE: Journal

LANGUAGE: English

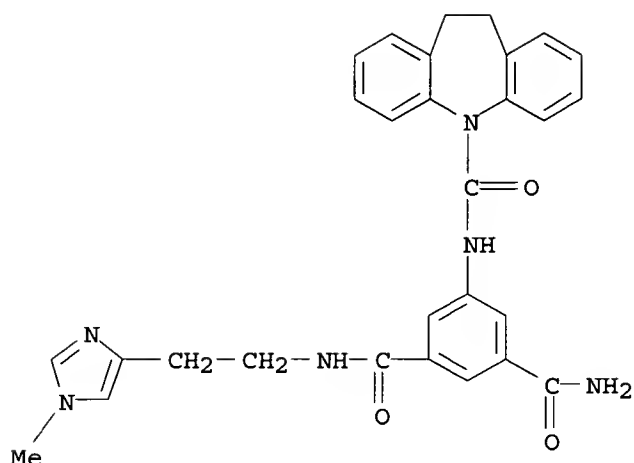
AB Chem. strategies are described for the design and automated high throughput synthesis of probe libraries of individual small mols. suitable for optimization into novel, potent, selective and orally bioavailable enzyme inhibitors. These libraries were directed towards serine proteases and were designed to incorporate novel scaffolds, structural diversity and other pharmacophoric features that served as peptide backbone replacements. The solid phase synthesis of probe libraries based on aryl scaffolds contg. amides, sulfonamides, sulfonates, ureas, and guanidines are described. Screening of the libraries against a series of serine proteases including thrombin and factor Xa produced a no. of useful hits appropriate for further optimization.

IT 208756-16-5P

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)  
(serine proteases-directed small mol. probe libraries)

RN 208756-16-5 CAPLUS

CN 1,3-Benzenedicarboxamide, 5-[[[(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)carbonyl]amino]-N-[2-(1-methyl-1H-imidazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:394320 CAPLUS

DOCUMENT NUMBER: 129:54189

TITLE: Aminobenzenedicarboxylic acid-based combinatorial libraries for discovery of protease inhibitors

INVENTOR(S): Graybill, Todd L.; Wu, Zhengdong; Subasinghe, Nalin; Fedde, Cynthia L.; Salvino, Joseph M.

PATENT ASSIGNEE(S): Graybill, Todd L., USA; Wu, Zhengdong; Subasinghe, Nalin; Fedde, Cynthia L.; Salvino, Joseph M.

SOURCE: PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

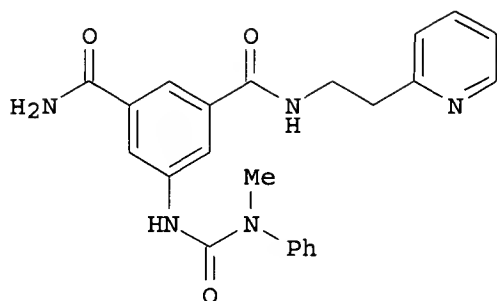
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

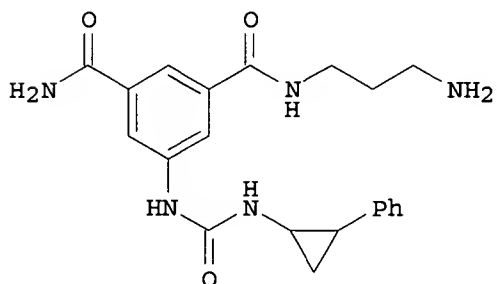
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9824760	A1	19980611	WO 1997-US21648	19971126
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9876242	A1	19980629	AU 1998-76242	19971126
US 6127191	A	20001003	US 1997-980062	19971126
PRIORITY APPLN. INFO.:			US 1996-32284P	P 19961203
			WO 1997-US21648	W 19971126
OTHER SOURCE(S):		CASREACT 129:54189; MARPAT 129:54189		
GI				





I



II

AB The invention provides a library of compds. contg. a common aminobenzenedicarboxylic acid core structure (scaffold) which serves as a template for synthesizing approx. 101-106 compds. which are analogs of the scaffold. The library is employed to study ligand binding by biol. receptors, such as enzymes, G-protein coupled receptors and membrane channels. For example, certain individual compds. within the library selectively bind and inhibit the action of trypsin-like serine proteases (no data). The invention also provides combinatorial synthetic methods for making such libraries. Addnl., the invention relates to novel scaffold-modified solid supports, esp. resins, and methods for prepg. them. Further, the invention is directed to screening methods, which comprise use of the compds. in suitable pharmaceutical assays. For instance, an Fmoc-protected Rink amide MBHA resin was deprotected, coupled with mono-Me 5-nitroisophthalate as a scaffold precursor, and reduced with  $\text{SnCl}_2$  to give an amino ester resin. This was submitted to a sequence of reaction with triphosgene, amination to give a urea, ester hydrolysis, acid activation, amidation, and  $\text{CF}_3\text{CO}_2\text{H}$  clip. One obtained sublibrary (14 compds.) included compds. I and II.

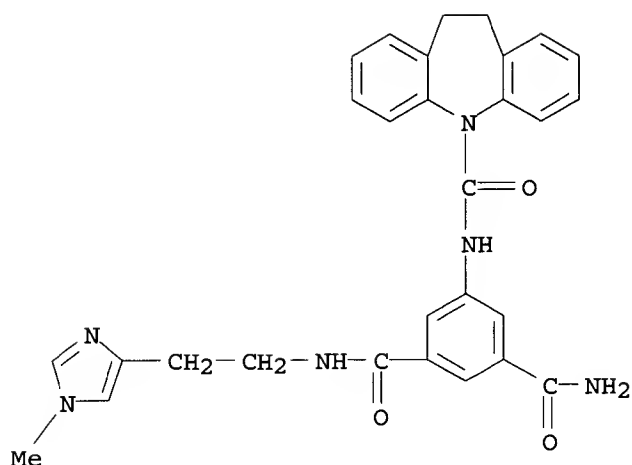
IT **208756-16-5P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminobenzenedicarboxylic acid-based combinatorial libraries for discovery of protease inhibitors)

RN 208756-16-5 CAPLUS

CN 1,3-Benzenedicarboxamide, 5-[[[(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)carbonyl]amino]-N-[2-(1-methyl-1H-imidazol-4-yl)ethyl]]- (9CI) (CA INDEX NAME)



L4 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:239217 CAPLUS

DOCUMENT NUMBER: 128:294711

TITLE: Preparation of N-substituted azaheterocyclic compounds as analgesics and antiinflammatories

INVENTOR(S): Jorgensen, Tine Krogh; Hohlweg, Rolf; Madsen, Peter; Andersen, Knud Erik; Treppendahl, Svend; Olsen, Uffe Bang; Polivka, Zdenek; Silhankova, Alexandra; Sindelar, Karel; Valenta, Vladimir; Kalisz, Tomas

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

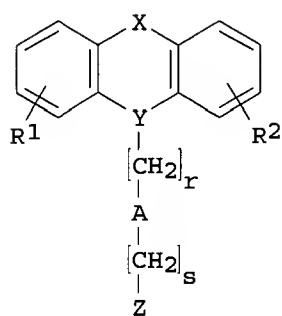
DOCUMENT TYPE: Patent

LANGUAGE: English

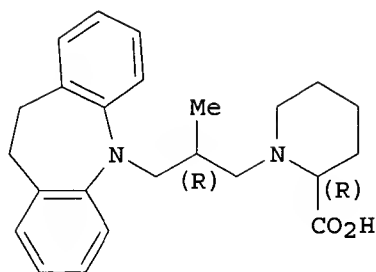
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815546	A1	19980416	WO 1997-DK421	19971002
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9743771	A1	19980505	AU 1997-43771	19971002
AU 741839	B2	20011213		
EP 934306	A1	19990811	EP 1997-941883	19971002
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9712202	A	19990831	BR 1997-12202	19971002
CN 1234797	A	19991110	CN 1997-199183	19971002
JP 2001501629	T2	20010206	JP 1998-517092	19971002
NO 9901563	A	19990603	NO 1999-1563	19990330
KR 2000048909	A	20000725	KR 1999-702939	19990403
PRIORITY APPLN. INFO.:			DK 1996-1089	A 19961004
			WO 1997-DK421	W 19971002
OTHER SOURCE(S):		MARPAT 128:294711		
GI				



I



II

AB The title compds. [I; R1, R2 = H, halo, CF3, etc.; X = o-phenylene, O, S, etc.; Y = N, CH, N(C=O), C:C(R8) (only first atom participates in the ring system and R8 = H, C1-6 alkyl); A = C.tplbond.C, C(O), C:CH, etc.; r, s = 0-4; Z = substituted piperidino, piperazino, pyrrolidino, etc.] and their salts, useful for the clin. treatment of painful, hyperalgesic and/or inflammatory conditions in which C-fibers play a pathophysiol. role by eliciting neurogenic pain or inflammation as well as useful for treatment of indications caused by or related to secretion and circulation of insulin antagonizing peptides, were prepd. and formulated. Thus, reaction of iminodibenzyl with [3-bromo-2(R)-methylpropoxy]tetrahydropyran in the presence of NaNH2 in C6H6 followed by methanesulfonylation of the resulting 3-(10,11-dihydro-5H-dibenzo[b,f]azepin-5-yl)-(2S)-methyl-1-propanol, reaction of the methanesulfonate with (R)-2-piperidinecarboxylic acid Et ester hydrochloride in the presence of K2CO3 in DMF, and hydrolysis of the resulting ester with 5N NaOH afforded the title compd. II.HCl with showed 47% inhibition of histamine induced pain response at 1.0 mg/kg.

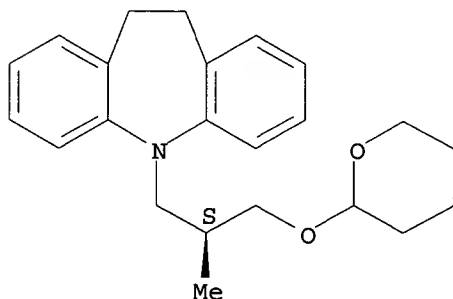
IT 205983-21-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of N-substituted azaheterocyclic compds. as analgesics and antiinflammatories)

RN 205983-21-7 CAPLUS

CN 5H-Dibenz[b,f]azepine, 10,11-dihydro-5-[2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]propyl]-, [2(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:723615 CAPLUS

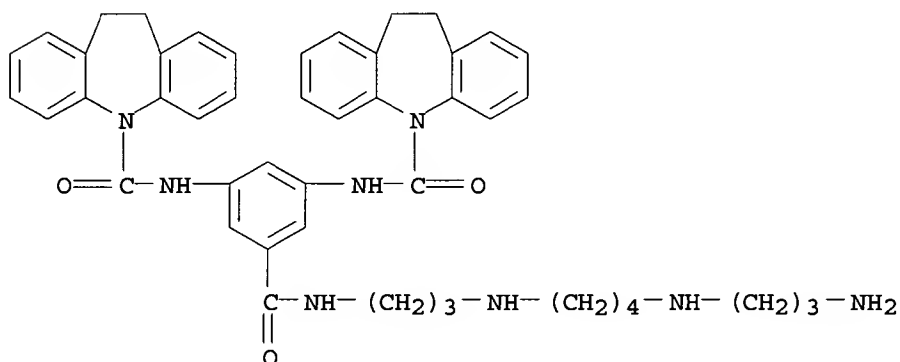
DOCUMENT NUMBER: 128:23122

TITLE: Structure-binding relation of philanthotoxins from  
nicotinic acetylcholine receptor binding assay

AUTHOR(S): Nakanishi, Koji; Huang, Xuefei; Jiang, Hong; Liu,  
Ying; Fang, Kan; Huang, Danwen; Choi, Seok-Ki; Katz,

09/ 995,324

CORPORATE SOURCE: Elizabeth; Eldefrawi, Mohyee  
Department of Chemistry, Columbia University, New  
York, NY, 10027, USA  
SOURCE: Bioorg. Med. Chem. (1997), 5(10), 1969-1988  
CODEN: BMECEP; ISSN: 0968-0896  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Philanthotoxins are noncompetitive inhibitors of the nicotinic  
acetylcholine receptor and the various glutamate receptors. Analogs  
carrying photoaffinity labels, fluorine atoms for solid-state NMR studies  
of ligand/receptor interaction, and large head groups such as porphyrins  
and planar bulky arom. rings (BIG analogs) for clarifying mode of entry  
and orientation of analogs in receptors have been synthesized, assayed  
against the nicotinic acetylcholine receptor, and brief comments are given  
for the assay results.  
IT 175085-76-4  
RL: BAC (Biological activity or effector, except adverse); BIOL  
(Biological study)  
(prepn. and structure-binding relationships of philanthotoxins from  
nicotinic acetylcholine receptor binding assay)  
RN 175085-76-4 CAPLUS  
CN 5H-Dibenz[b,f]azepine-5-carboxamide, N,N'-[5-[[[3-[[4-[(3-  
aminopropyl)amino]butyl]amino]propyl]amino]carbonyl]-1,3-  
phenylene]bis[10,11-dihydro- (9CI) (CA INDEX NAME)



L4 ANSWER 19 OF 96 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1997:568120 CAPLUS  
DOCUMENT NUMBER: 127:234258  
TITLE: Indoliny- and tetrahydroquinolylcarboxamidines with  
anticonvulsant activity  
INVENTOR(S): Reddy, N. Laxma; Maillard, Michael; Berlove, David;  
Magar, Sharad; Durant, Graham J.  
PATENT ASSIGNEE(S): Cambridge Neuroscience, Inc., USA; Reddy, N. Laxma;  
Maillard, Michael; Berlove, David; Magar, Sharad;  
Durant, Graham J.  
SOURCE: PCT Int. Appl., 103 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730054	A1	19970821	WO 1997-US2678	19970214

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9722780 A1 19970902 AU 1997-22780 19970214

AU 733475 B2 20010517

EP 925300 A1 19990630 EP 1997-906923 19970214

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI

JP 2000504730 T2 20000418 JP 1997-529602 19970214

US 6358993 B1 20020319 US 1999-425582 19991022

PRIORITY APPLN. INFO.:

US 1996-601992 A 19960215

WO 1997-US2678 W 19970214

US 1997-858399 A3 19970519

OTHER SOURCE(S): MARPAT 127:234258

AB Title compds. (>250 compds.) were prepd. Thus, 1-aminonaphthalene was treated with BrCN to give 1-naphtylcyanamide which was treated with indolin mesylate to give N-(1-naphthyl)-1-indolinylcarboxamidine (I). I at 2 mg/kg i.p. caused 82% inhibition of audiogenic seizures in mice. The title compds. are particularly useful for the treatment or prophylaxis of neurol. injury and neurodegenerative disorders.

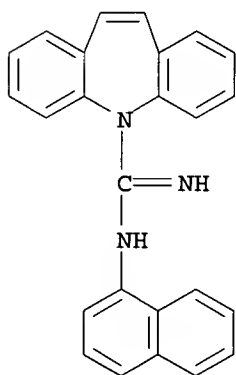
IT 195437-37-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of indolinyl- and tetrahydroquinolylcarboxamidines with anticonvulsant activity)

RN 195437-37-7 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboximidamide, N-1-naphthalenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 20 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:545505 CAPLUS

DOCUMENT NUMBER: 127:229173

TITLE: Characterization of carbamazepine metabolism in a mouse model of carbamazepine teratogenicity

AUTHOR(S): Amore, Benny M.; Kalhorn, Thomas F.; Skiles, Gary L.; Hunter, Ann P.; Bennett, Greg D.; Finnell, Richard H.;

Nelson, Sidney D.; Slattery, John T.  
 CORPORATE SOURCE: Department of Pharmaceutics, School of Pharmacy,  
 University of Washington, Seattle, WA, 98195-7610, USA  
 SOURCE: Drug Metab. Dispos. (1997), 25(8), 953-962  
 CODEN: DMDSAI; ISSN: 0090-9556  
 PUBLISHER: Williams & Wilkins  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

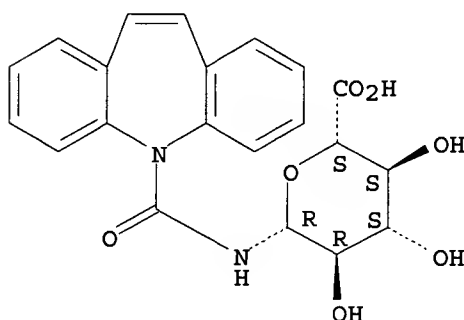
AB The disposition of carbamazepine (CBZ) was investigated in the SWV mouse. A 14C-CBZ dose was administered to CBZ pretreated mice, and the distribution of radiolabeled material was detd. Twenty-four hours after the 14C-CBZ dose, 92.5% of the dose was accounted for in urine (56%), in the viscera and carcass (22%), in feces (11%), and expired as 14CO2 (2%). CBZ metabolites present in hydrolyzed urine were also identified using a combination of spectroscopic techniques. CBZ, CBZ-10,11-epoxide (CBZE), 2-and 3-hydroxy-CBZ, methylsulfonyl-CBZ, and glucuronides of CBZ and CBZE accounted for 64% of total urinary radioactivity (0-24 h) in CBZ pretreated mice. Minor metabolites of CBZ included novel cysteine and N-acetylcysteine conjugates of CBZ, as well as a methylsulfonyl conjugate of CBZE not previously reported. The urinary excretion of these thioether conjugates was increased in CBZ/phenobarbital pretreated mice and decreased in CBZ/stiripentol pretreated mice in comparison with CBZ-only treated mice. Preliminary studies of the effects of phenobarbital and stiripentol on the urinary abundance of these metabolites are consistent with the modulation of teratogenicity in the SWV mouse by the same pretreatments. These data suggest the formation of thioether metabolites of CBZ may be related to CBZ teratogenicity in the SWV mouse.

IT 60342-79-2, Carbamazepine N-glucuronide  
 RL: ADV (Adverse effect, including toxicity); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
 (characterization of carbamazepine metab. in model of carbamazepine teratogenicity)

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 21 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:537574 CAPLUS

DOCUMENT NUMBER: 127:161697

TITLE: 2-Amino heterocycles and their therapeutic uses as leukotriene biosynthesis inhibitors

INVENTOR(S): Es-Sayed, Mazen; Yamamoto, Masaru; Frobels, Klaus; Poll, Chris; Grix, Suzanna; Tudhope, Stephen

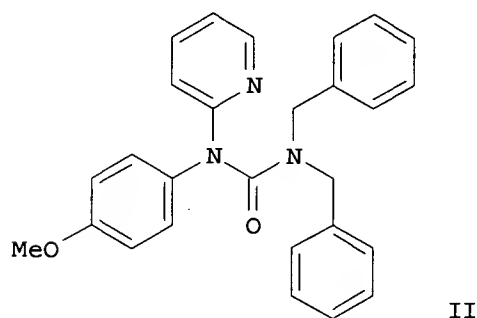
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany; Es-Sayed, Mazen; Yamamoto, Masaru; Frobels, Klaus; Poll, Chris; Grix, Suzanna; Tudhope, Stephen

SOURCE: PCT Int. Appl., 275 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9724328	A1	19970710	WO 1996-EP5643	19961216
W: AU, BG, BR, BY, CA, CN, CZ, EE, HU, IL, IS, JP, KE, KP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9713728	A1	19970728	AU 1997-13728	19961216
PRIORITY APPLN. INFO.:			GB 1995-26560	19951227
			WO 1996-EP5643	19961216
OTHER SOURCE(S):			MARPAT 127:161697	
GI				



AB 2-Amino heterocycles R<sub>1</sub>R<sub>2</sub>NCOR<sub>3</sub> [I; R<sub>1</sub> = H, Me, (un)substituted 6-membered arom. heterocycle contg. .ltoreq.2 N atoms and optionally benzo-fused; R<sub>2</sub> = (un)substituted adamantyl, cycloalkyl, pyridyl, Ph, CH<sub>2</sub>Ph, tetralin-5-yl, 2-norbornyl, 1-azabicyclo[2.2.2]oct-3-yl; or NR<sub>1</sub>R<sub>2</sub> forms .alpha.-carboline residue; R<sub>3</sub> = (un)substituted or cyclic amino groups linked via a bond, carbonyl, or alkylene group] are disclosed. I can be used for the prodn. of medicaments which inhibit leukotriene synthesis (in particular LTB<sub>4</sub>), and are esp. useful for the treatment and control of respiratory diseases and inflammatory processes (no data). For instance, condensation of 2-chloropyridine with 4-MeOC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> at 150.degree. gave 2-(4-methoxyanilino)pyridine, which reacted with ClCO<sub>2</sub>CCl<sub>3</sub> and then HN(CH<sub>2</sub>Ph)<sub>2</sub> in dioxane at 60.degree. to give title compd. II plus a byproduct.

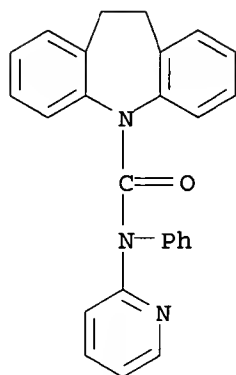
IT 193555-04-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 2-amino heterocycles as leukotriene biosynthesis inhibitors)

RN 193555-04-3 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-N-phenyl-N-2-pyridinyl- (9CI) (CA INDEX NAME)



L4 ANSWER 22 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1997:347198 CAPLUS  
 DOCUMENT NUMBER: 127:4949  
 TITLE: Synthetic and Mechanistic Studies on the  
 Azabicyclo[7.3.1]enediyne Core and  
 Naphtho[2,3-h]quinoline Portions of Dynemicin A  
 AUTHOR(S): Magnus, Philip; Eisenbeis, Shane A.; Fairhurst, Robin  
 A.; Iliadis, Theodore; Magnus, Nicholas A.; Parry,  
 David  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University  
 of Texas at Austin, Austin, TX, 78712, USA  
 SOURCE: J. Am. Chem. Soc. (1997), 119(24), 5591-5605  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The synthesis of the 13-keto-10-azabicyclo[7.3.1]enediyne core structure of dynemicin A has been achieved by two routes. The chem. of the 13-keto core structure is dominated by the unusually facile bridgehead enolization. Comparison of the rates of cycloaromatization of a variety of enediynes revealed that substantial rate differences occurred even though the distance between the bonding acetylenes was virtually identical. A nonradical cycloaromatization pathway, initiated by thiol addn. to the enediyne system, was discovered, and the simple core amine I exhibits modest in vitro and in vivo antitumor activity. Finally, two methods for the synthesis of the naphtho[2,3-h]quinoline portion of dynemicin A are described, and both these compds., II [R = COCMe<sub>3</sub>, Et], also exhibit antitumor activity.

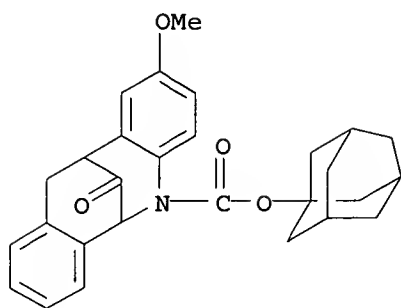
IT 159258-11-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and antitumor activity of the azabicyclohexadecatetraenediyne and naphthoquinoline fragments of dynemicin A)

RN 159258-11-4 CAPLUS

CN 6,12-Methanodibenz[b,f]azocine-5(6H)-carboxylic acid, 11,21-dihydro-2-methoxy-13-oxo-, tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl ester (9CI) (CA INDEX NAME)





L4 ANSWER 23 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:193424 CAPLUS

DOCUMENT NUMBER: 126:271750

TITLE: Characterization of the metabolites of carbamazepine in patient urine by liquid chromatography/mass spectrometry

AUTHOR(S): Maggs, J. L.; Pirmohamed, M.; Kitteringham, N. R.; Park, B. K.

CORPORATE SOURCE: Department of Pharmacology and Therapeutics, University of Liverpool, Liverpool, L69 3BX, UK

SOURCE: Drug Metab. Dispos. (1997), 25(3), 275-280

CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The urinary metabolites of carbamazepine (CBZ) in epileptic patients receiving long-term drug treatment have been characterized by LC/MS. CBZ-10,11-epoxide (9.6-15.0 .mu.g/mL), trans-10,11-dihydrodiol-CBZ (273.0-400.00 .mu.g/mL), and CBZ (2.4-3.8 .mu.g/mL) were measured by HPLC. The secondary N-glucuronide of CBZ, four phenolic O-glucuronides (including those of 2- and 3-OH-CBZ), two addnl. OH-CBZ O-glucuronides, and the N-glucuronide of CBZ-10,11-epoxide constituted the products of either direct conjugation or preliminary monooxygenation. Derivs. of these monooxygenated compds., which were characterized as O-glucuronides, were represented by dihydroxylated (catechol) CBZ and its putative O-Me metabolite and by 10,11-dihydrodiol-CBZ. 10,11-Dihydro-10-OH-CBZ O-glucuronide, a metabolite thought to be excreted only by uremic subjects, was not found. More complicated biotransformations of the 10,11-ene moiety were revealed by two carbinol products of azepine ring contraction: 9-OH-methyl-10-carbamoyl acridan and an hydroxylated deriv. thereof, which were excreted as O-glucuronides. No polar sulfur-contg. metabolites that might serve as indicators of reactive intermediate formation were found in human urine.

IT 60342-79-2

RL: ANT (Analyte); MFM (Metabolic formation); ANST (Analytical study);

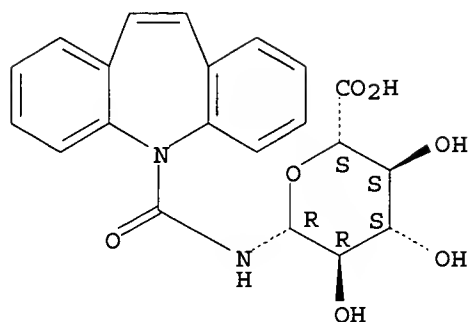
BIOL (Biological study); FORM (Formation, nonpreparative)

(characterization of metabolites of carbamazepine in human urine by liq. chromatog./mass spectrometry)

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 24 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:708300 CAPLUS

DOCUMENT NUMBER: 125:328528

TITLE: Preparation of heterocyclic tricyclic analgesics, antidiabetics and antiinflammatory agents

INVENTOR(S): Madsen, Peter; Andersen, Knud Erik; Doerwald, Florenzio Zaragossa; Joergensen, Tine Krogh; Andersen, Henrik Sune; Hohlweg, Rolf; Olsen, Uffe Bang

PATENT ASSIGNEE(S): Novo Nordisk A/s, Den.

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

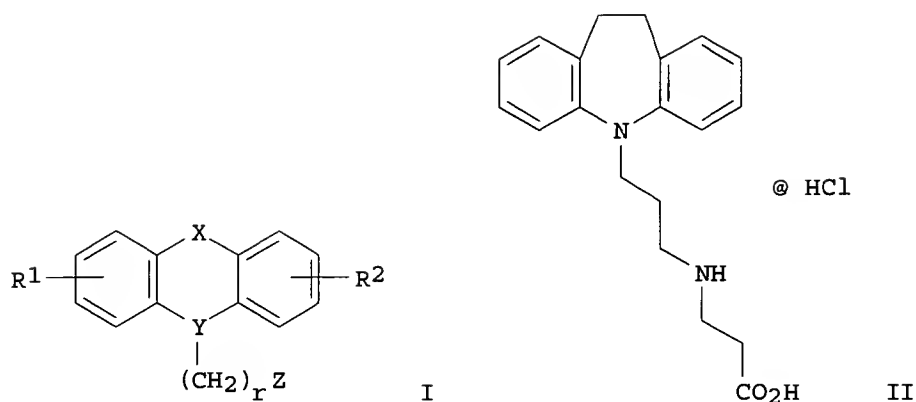
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9631481	A1	19961010	WO 1996-DK141	19960401
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML				
US 5962449	A	19991005	US 1996-623447	19960328
CA 2217198	AA	19961010	CA 1996-2217198	19960401
AU 9652706	A1	19961023	AU 1996-52706	19960401
EP 820443	A1	19980128	EP 1996-909078	19960401
EP 820443	B1	20010919		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 11503129	T2	19990323	JP 1996-529870	19960401
AT 205833	E	20011015	AT 1996-909078	19960401
ZA 9602733	A	19961024	ZA 1996-2733	19960404
PRIORITY APPLN. INFO.:			DK 1995-407	A 19950407
			DK 1995-1002	A 19950911
			WO 1996-DK141	W 19960401
OTHER SOURCE(S):		MARPAT 125:328528		
GI				



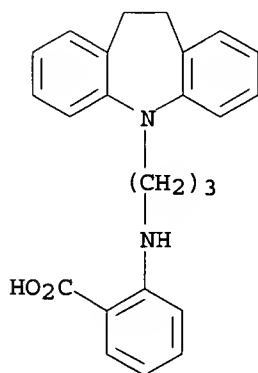
AB The title compds. [I; R1, R2 = H, halogen, CF<sub>3</sub>, OH, alkyl, alkoxy; X = O, S, CH<sub>2</sub>CH<sub>2</sub>, (un)substituted NH, CH<sub>2</sub>O, OCH<sub>2</sub>, S(:O), etc.; Y = NCH<sub>2</sub>, CHCH<sub>2</sub>, C:CH; Z = (un)substituted 2-pyridylamino, (un)substituted cyclohexylamino, etc.; r = 1-3], useful for the clin. treatment of painful, hyperalgesic and/or inflammatory conditions in which C-fibers play a pathophysiol. role by eliciting neurogenic pain or inflammation, and for the treatment of noninsulin-dependent diabetes mellitus (no data), are prepd. and a I-contg. formulation presented. Thus, dihydrodibenz[b,f]azepine II (m.p. 114-117.degree.) was prepd. in 4 steps from 10,11-dihydro-5H-dibenz[b,f]azepine and demonstrated a 36% inhibition of pain in a mouse formalin-induced pain model at 0.1 mg/kg.

IT **183476-83-7P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of heterocyclic tricyclic analgesics, antidiabetics and antiinflammatory agents)

RN 183476-83-7 CAPLUS

CN Benzoic acid, 2-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]amino]-  
(9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 96 CAPLUS COPYRIGHT 2002 ACS

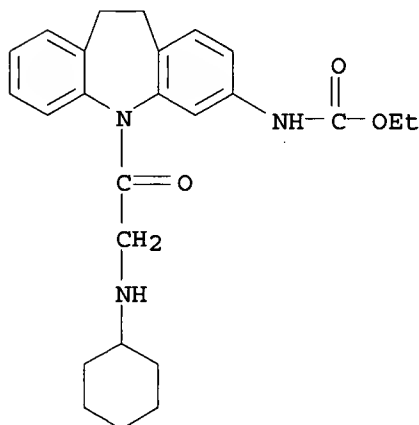
ACCESSION NUMBER: 1996:464304 CAPLUS

DOCUMENT NUMBER: 125:75929

TITLE: 3-Alkoxy-carbonylamino-5-(aminoacyl)dibenz[b,f]azepines and their antiarrhythmic activity

AUTHOR(S): Skoldinov, A. P.; Kaverina, N. V.; Gritsenko, A. N.;  
Lyskovtsev, V. V.; Turilova, A. I.; Vunderlikh, Kh.;

Shtark, A.; Poppe, Kh.; Barch, R.; et al.  
 CORPORATE SOURCE: Institut Farmakologii, Moscow, Russia  
 SOURCE: Khim.-Farm. Zh. (1996), 30(3), 26-30  
 CODEN: KHFZAN; ISSN: 0023-1134  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB A series of 37 3-alkoxycarbonyl-5-monoalkylaminoacyl derivs. of dibenz[b,f]azepines was prepd. Almost all of the compds. showed considerable antiarrhythmic effect in animal expts. The mol. structure-biol. activity relationship is discussed.  
 IT **134068-22-7P**  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. and antiarrhythmic activity of dibenzazepines)  
 RN 134068-22-7 CAPLUS  
 CN Carbamic acid, [5-[(cyclohexylamino)acetyl]-10,11-dihydro-5H-dibenz[b,f]azepin-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 26 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1996:241480 CAPLUS  
 DOCUMENT NUMBER: 124:331579  
 TITLE: Bioactivation of carbamazepine in the rat in vivo.  
 Evidence for the formation of reactive arene oxide(s)  
 AUTHOR(S): Madden, Stephen; Maggs, James L.; Park, B. Kevin  
 CORPORATE SOURCE: Department Pharmacology, University Liverpool,  
 Liverpool, L69 3BX, UK  
 SOURCE: Drug Metab. Dispos. (1996), 24(4), 469-79  
 CODEN: DMDSAI; ISSN: 0090-9556  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The metab. of carbamazepine (CBZ) and its major metabolite in humans, carbamazepine 10,11-epoxide (CBZ-E), was examd. in the rat in vivo. Particular emphasis was placed on the identification of dihydrohydroxythio adducts, which are detoxication products of reactive arene oxide intermediates. Anesthetized and cannulated male Wistar rats were administered [3H]CBZ (25 .mu.g.cntdot.kg-1 or 25 mg.cntdot.kg-1) or [3H]CBZ-E (25 .mu.g.cntdot.kg-1 or 25 mg.cntdot.kg-1) i.v. and bile and urine collected for 5 h. Less than 8% of drug was excreted in the urine for each dosing regimen. Biliary excretion accounted for 73.7 and 41.8% of administered CBZ (25 .mu.g.cntdot.kg-1 and 25 mg.cntdot.kg-1, resp.) and 47.6 and 28.1% of administered CBZ-E (25 .mu.g.cntdot.kg-1 and 25 mg.cntdot.kg-1, resp.). The major route of metab. of both CBZ and CBZ-E was N-glucuronidation. In rats given CBZ (25 mg.cntdot.kg-1), the

N-glucuronide of the parent compd. accounted for 12.6% of the dose, whereas CBZ-E N-glucuronide accounted for 12.3% of the dose. At the lower dose of 25 .mu.g.cntdot.kg-1, these accounted for 18.6 and 36.7% of the dose, resp. Similarly, for rats given CBZ-E (25 mg.cntdot.kg-1), the N-glucuronide of the parent compd. was the major metabolite, accounting for 19.1% of the dose. O-glucuronides were relatively minor metabolites of both drugs. Glutathione adducts were identified in the bile of both groups of animals. Although these adducts were relatively minor metabolites of CBZ-E (1.8% of the dose), they were more substantial products of the metab. of CBZ. Three isomeric glutathionyl dihydrohydroxy-CBZ adducts were identified by LC/MS. They collectively accounted for 5.8% of the dose. In conclusion, we have provided evidence, in rats, for the generation of a reactive arene oxide species from CBZ. If not adequately detoxified, via conjugation with glutathione, this has the potential to initiate cellular damage. In humans, a similar mechanism may be involved in CBZ-assocd. hypersensitivity.

IT 60342-79-2, Carbamazepine N-glucuronide

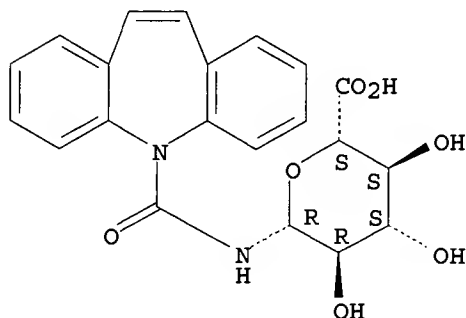
RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(bioactivation of carbamazepine in rat in vivo. Evidence for formation of reactive arene oxide(s))

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:97032 CAPLUS

DOCUMENT NUMBER: 124:260666

TITLE: Synthesis of philanthotoxin analogs with bulky heads including porphyrins. Self-assembly monitored by circular dichroism

AUTHOR(S): Huang, Danwen; Matile, Stefan; Berova, Nina; Nakanishi, Koji

CORPORATE SOURCE: Dep. Chem., Columbia Univ., New York, NY, 10027, USA

SOURCE: Heterocycles (1996), 42(2), 723-36

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Philanthotoxin (PhTX) analogs, e.g. I [R = NH(CH<sub>2</sub>)<sub>3</sub>NH(CH<sub>2</sub>)<sub>4</sub>NH(CH<sub>2</sub>)<sub>3</sub>NH<sub>2</sub>, NH(CH<sub>2</sub>)<sub>3</sub>NH(CH<sub>2</sub>)<sub>4</sub>NH(CH<sub>2</sub>)<sub>3</sub>NH(CH<sub>2</sub>)<sub>4</sub>NH<sub>2</sub>, NH(CH<sub>2</sub>)<sub>3</sub>NH(CH<sub>2</sub>)<sub>4</sub>NH(CH<sub>2</sub>)<sub>3</sub>NHCOCH(NH<sub>2</sub>)(C

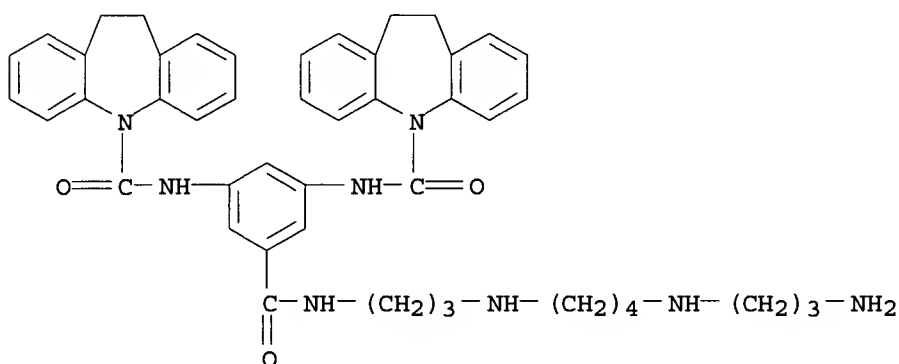
H2) 3NHC (:NH) NH2, NH(CH2) 5CONH(CH2) 3NH(CH2) 4NH(CH2) 3COCH(NH2) (CH2) 3NH (:NH) N H2] and II (R1 = R2, X = CH, M = H; R = R2, X = N, M = Zn) with bulky bis-iminodibenzyl and porphyrin head groups have been prepd. Exciton coupled CD studies show that dependent on the hydrophobicity of the head group PhTX analogs may get amphiphilic properties forming micelles in aq. soln.

IT 175085-76-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and exciton coupled CD studies of amphiphilic properties of philanthotoxin analogs)

RN 175085-76-4 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, N,N'-[5-[[[3-[[4-[(3-aminopropyl)amino]butyl]amino]propyl]amino]carbonyl]-1,3-phenylene]bis[10,11-dihydro- (9CI) (CA INDEX NAME)



L4 ANSWER 28 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:647100 CAPLUS

DOCUMENT NUMBER: 123:101949

TITLE: N+-Glucuronidation of aliphatic tertiary amines in human: antidepressant versus antipsychotic drugs

AUTHOR(S): Luo, H.; Hawes, E. M.; McKay, G.; Korchinski, E. D.; Midha, K. K.

CORPORATE SOURCE: College of Pharmacy and Nutrition and College of Medicine, University of Saskatchewan, Saskatoon, SK, S7N 0W0, Can.

SOURCE: Xenobiotica (1995), 25(3), 291-301

CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Metabolic N+-glucuronidation of aliph. tertiary amine antidepressant or antipsychotic drugs was investigated in man. In each case, urine was collected either from patients and/or from healthy volunteers who were administered the drug orally. Metabolites were sep'd. by hplc and individually collected prior to mass spectrometric anal. in the fast atom bombardment mode. The structure of each metabolite identified as a quaternary ammonium-linked glucuronide metabolite was confirmed by direct comparison of its mass spectrum and chromatog. behavior with that of an authentic std. synthesized in these labs. Of the 10 antipsychotic drugs exam'd. clozapine and loxapine were the only two for which the N+-glucuronidation pathway was obs'd., whereas all four antidepressants gave the resp. N+-glucuronide metabolite. The N+-glucuronide metabolites in 24 h urine samples were quantified by hplc. The mean (n = 3) percentage of the dose excreted as the metabolite was found to be 1.6 and 3.1% in the cases of the antipsychotic agents loxapine and clozapine resp., whereas for the antidepressants clomipramine, imipramine, trazodone

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and trimipramine these means varied between 0.1 and 0.8%.

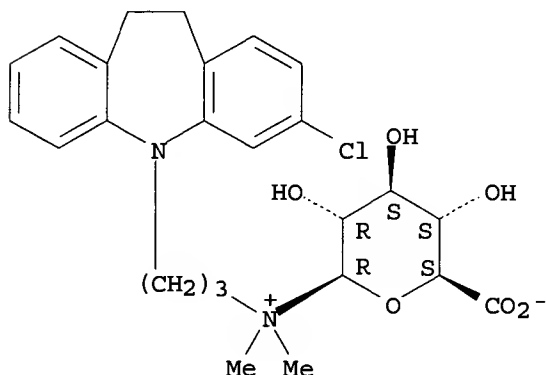
IT 165602-83-5, Clomipramine N-glucuronide  
RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(N+-glucuronidation of aliph. tertiary amine antidepressants and antipsychotics in humans)

RN 165602-83-5 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanaminium, 3-chloro-N-.beta.-D-glucopyranuronosyl-10,11-dihydro-N,N-dimethyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 29 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:25986 CAPLUS

DOCUMENT NUMBER: 122:9266

TITLE: Relative rates of cycloaromatization of dynemicin azabicyclo[7.3]enediynes core structures. An unusual change in .DELTA.S.thermod.

AUTHOR(S): Magnus, Philip; Fairhurst, Robin A.

CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Texas, Austin, TX, 78712, USA

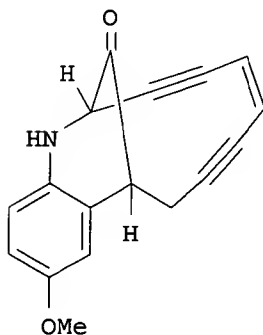
SOURCE: J. Chem. Soc., Chem. Commun. (1994), (13), 1541-2

CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

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AB A series of dynemicin core azabicyclo[7.3]enediynes undergo cycloaromatization at dramatically different rates despite the fact that the distance (r, by x-ray diffraction) between the bonding acetylenes is

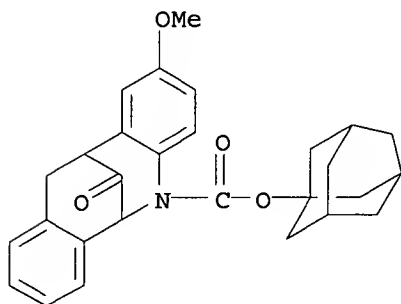
practically identical (3.4 .ANG.); when the carbamate protecting group is removed to give the sec-amine I, it cycloaromatizes more rapidly, and the entropy of activation changes from a neg. to pos.

IT **159258-11-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and redn. of)

RN 159258-11-4 CAPLUS

CN 6,12-Methanodibenz[b,f]azocine-5(6H)-carboxylic acid, 11,21-dihydro-2-methoxy-13-oxo-, tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl ester (9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:680471 CAPLUS

DOCUMENT NUMBER: 121:280471

TITLE: Preparation of dynemicin analogs as bactericides and antitumor agents

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wenderborn, Sebastian V.; Nicolaou, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Min; Maligres, Peter E.; Suzuki, Toshio

PATENT ASSIGNEE(S): Scripps Research Institute, USA

SOURCE: U.S., 114 pp. Cont.-in-part of U.S.Ser. No. 886,984, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5281710	A	19940125	US 1992-939104	19920901
US 5276159	A	19940104	US 1992-886984	19920521
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-US4708	19930518
W: AU, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343807	A1	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-913966	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07508037	T2	19950907	JP 1993-503816	19930518
US 5527805	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118

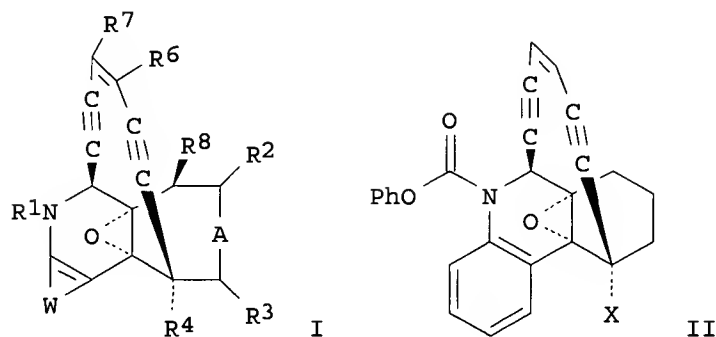
PRIORITY APPLN. INFO.:

US 1990-562269	19900801
US 1991-673199	19910321
US 1991-734613	19910723
US 1991-788225	19911105



US 1992-886984 19920521  
 US 1992-939104 19920901  
 WO 1993-US4708 19930518

OTHER SOURCE(S) : MARPAT 121:280471  
 GI



AB The title compds. I [A = double or single bond; R1 = H, alkyl, phoxycarbonyl, etc.; R2 = H, carboxyl, hydroxymethyl, etc.; R3 = H, alkoxy; R4 = H, hydroxyl, alkoxy, etc.; R6 and R7 are each H or together with the intervening vinylene group form a one, two or three fused arom. six-membered ring system; W together with the bonded, intervening, vinylene group (i.e., the unsatd. carbon atoms bonded to W) forms a substituted arom. hydrocarbyl ring system contg. 1, 2, or 3 six-membered rings such that said fused ring compd. contains 3, 4, or 5 fused 6-membered rings all but two of which rings are arom., and in which that arom. hydrocarbyl ring system, W, is joined [a,b] to the structure shown; R8 = H, or Me; a proviso is given] are prepd. Title compd. II (X = OH) (prepn. given) in vitro exhibited IC50 of  $6.3 \times 10^{-6}$  M against a variety of cancer cell lines. II (X = H) in vitro exhibited IC50 of  $5.0 \times 10^{-6}$  M against a variety of cancer cell lines.

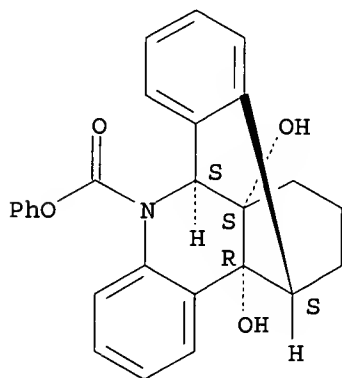
IT 130012-98-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and reaction of, in prepn. of bactericide and antitumor agent)

RN 130012-98-5 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
 11,12-dihydro-12,13-dihydroxy-, phenyl ester,  
 (6.alpha.,11.alpha.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 31 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:680470 CAPLUS

DOCUMENT NUMBER: 121:280470

TITLE: Preparation of dynemicin analogs as DNA binding, antibiotic, and antitumor agents.

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wendeborn, Sebastian V.; Nicolaou, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Min; Maligres, Peter E.; Suzuki, Toshio

PATENT ASSIGNEE(S): Scripps Research Institute, USA

SOURCE: U.S., 109 pp. Cont.-in-part of U.S. Ser. No. 788,225. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5276159	A	19940104	US 1992-886984	19920521
US 5281710	A	19940125	US 1992-939104	19920901
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-US4708	19930518
W: AU, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343807	A1	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-913966	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07508037	T2	19950907	JP 1993-503816	19930518
US 5527805	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118
PRIORITY APPLN. INFO.:			US 1990-562269	19900801
			US 1991-673199	19910321
			US 1991-734613	19910723
			US 1991-788225	19911105
			US 1992-886984	19920521
			US 1992-939104	19920901
			WO 1993-US4708	19930518
OTHER SOURCE(S):			MARPAT 121:280470	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [I; R1 = H, alkyl, PhO2C, PhCH2O2C, 9-fluorenylmethoxycarbonyl, o-nitrobenzyloxycarbonyl, (substituted) alkoxy carbonyl; R2 = H, CO2H, CH2OH, carbonyloxyalkyl; R3 = H, alkoxy; R4 = H, OH, alkoxy, oxyacetic acid, oxyacetic hydrocarbyl or benzyl ester, oxyacetic amide, acyloxy, etc.; R6, R7 = H; R6R7 = atoms to form a 1, 2, or 3-fused arom. 6-membered ring system; R8 = H, Me, with provisos; A = double or single bond; W = atoms to form an arom. hydrocarbyl ring system contg. 1, 2, or 3 six-membered rings such that the fused ring compd. contains 3, 4, or 5 fused rings, all but 2 of which are arom.], were prepd. Chimeric compds. having the fused ring system compd. as an aglycon bonded to (i) a sugar moiety as the oligosaccharide portion or (ii) a monoclonal antibody or antibody combining site portion thereof that immunoreacts with target tumor cells are also disclosed. Thus, title

compd. III (preparable via claimed compd. II) inhibited Molt-4 T-cell leukemia with  $IC_{50} = 2.0 \times 10^{-14}$  M; III was 1-8 orders of magnitude more active against tumor cells than against normal cells. I structure-activity relationships are discussed.

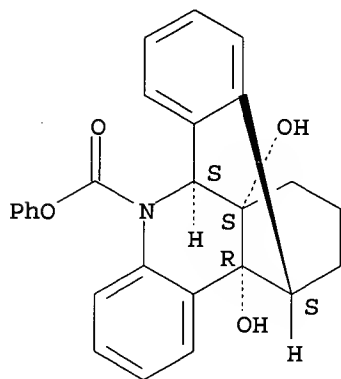
IT 130012-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 130012-98-5 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
11,12-dihydro-12,13-dihydroxy-, phenyl ester,  
(6.alpha.,11.alpha.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 32 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:217054 CAPLUS

DOCUMENT NUMBER: 120:217054

TITLE: Studies on dynemicin. A nonradical cycloaromatization pathway for the azabicyclo[7.3.1]enediynes core structure initiated by thiolate addition

AUTHOR(S): Magnus, Philip; Eisenbeis, Shane A.; Rose, William C.; Zein, Nada; Solomon, Wyle

CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Texas, Austin, TX, 78712, USA

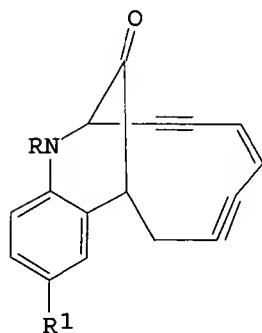
SOURCE: J. Am. Chem. Soc. (1993), 115(26), 12627-8

CODEN: JACSAT; ISSN: 0002-7863

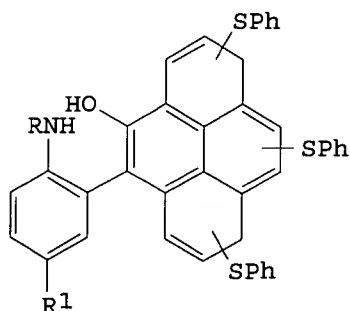
DOCUMENT TYPE: Journal

LANGUAGE: English

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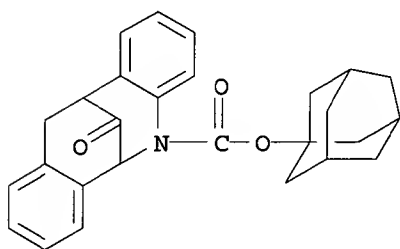
II

AB The azabicyclododecenediyne I (R = R1 = H) and its derivs. I (R = CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl, CO<sub>2</sub>Me, adamantyloxycarbonyl, R1 = H) undergo Bergman cycloaromatization via a polar, non-radical pathway. I (R = R1 = H, OMe) have antitumor activity in mice against P388 leukemia with T/C ratios of 175 and 170% resp. at 2mg/kg. I (R = R1 = H) was 350 times more potent than I (R = adamantyloxycarbonyl, R1 = H) against HCT116 human colon carcinoma, demonstrating that diradical formation is not required for antitumor activity.

IT **154126-03-1P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 154126-03-1 CAPLUS

CN 6,12-Methanodibenz[b,f]azocine-5(6H)-carboxylic acid, 11,12-dihydro-13-oxo-, tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl ester (9CI) (CA INDEX NAME)



L4 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:603206 CAPLUS

DOCUMENT NUMBER: 119:203206

TITLE: Molecular design, chemical synthesis, kinetic studies, calculations, and biological studies of novel enediynes equipped with triggering, detection, and deactivating devices. Model dynemicin A epoxide and cis-diol systems

AUTHOR(S): Nicolaou, K. C.; Dai, W. M.; Hong, Y. P.; Baldrige, K. K.; Siegel, J. S.; Tsay, S. C.

CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA

SOURCE: J. Am. Chem. Soc. (1993), 115(18), 7944-53  
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A series of enediyne model systems of the dynemicin A type equipped with triggering and modulating/signaling devices were designed, synthesized, and studied. Specifically, I (R = CO<sub>2</sub>Ph, CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>SO<sub>2</sub>Ph; R1R2 = H<sub>2</sub>, CH:CHCH:CH) were synthesized via ring closures involving intramol. acetylide addns. to carbonyl groups followed by deoxygenation. I (R = CO<sub>2</sub>Ph) underwent cycloaromatization to give diols II (R = CO<sub>2</sub>Ph) upon acid treatment. These conversions were obsd. with significant changes in the UV and fluorescence spectra of the compds. involved. I (R = CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>SO<sub>2</sub>Ph) upon activation with base (DBU or basic buffer soln.), were converted to I (R = H) which were further transformed into cis-diols III by exposure to silica gel in wet benzene. Kinetic studies used to det. the free energies of activation (.DELTA.G.dbldag.) for the

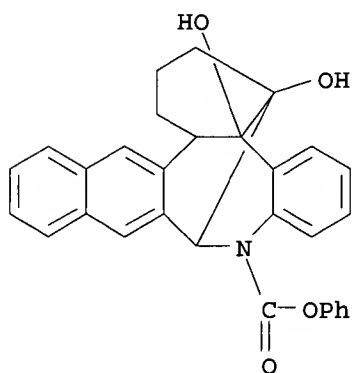
cycloaromatization of III ( $R_1, R_2 = H$ ) (22.6 kcal/mol, 30 .degree.) and III ( $R_1R_2 = CH:CHCH:CH$ ) (25.7 kcal/mol, 37 .degree.) to II ( $R = H$ ). Ab initio calcns. regarding the reactivity of these systems were in agreement with the exptl. findings. The isolation of III and II ( $R = H$ ) provide strong support for the postulated intermediates in the dynemicin A reaction cascade. Cytotoxicity data are reported for I ( $R = CO_2CH_2CH_2SO_2Ph$ ).

IT **137648-63-6P**

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in cycloaromatization of dynemicin model compd.)

RN 137648-63-6 CAPLUS

CN 13,6,14-[1]Butanyl[4]ylidenbenzo[b]naphth[2,3-f]azocine-5(6H)-carboxylic acid, 13,14-dihydro-14,15-dihydroxy-, phenyl ester,  
(6.alpha.,13.alpha.,14.beta.,15R\*)- (9CI) (CA INDEX NAME)



L4 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:102363 CAPLUS

DOCUMENT NUMBER: 118:102363

TITLE: Synthesis and characterization of quaternary ammonium-linked glucuronide metabolites of drugs with an aliphatic tertiary amine group

AUTHOR(S): Luo, H.; Hawes, E. M.; McKay, G.; Midha, K. K.

CORPORATE SOURCE: Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.

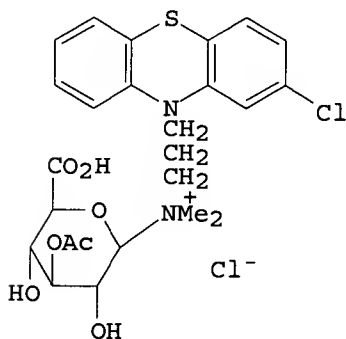
SOURCE: J. Pharm. Sci. (1992), 81(11), 1079-83

CODEN: JPMSAE; ISSN: 0022-3549

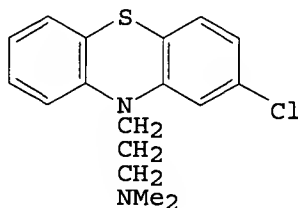
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB A synthetic approach was developed to make the quaternary ammonium-linked glucuronide metabolites, e.g., I, of compds., such as II, with aliph. tertiary amine group. The key step involved quaternization of the compd. with Me (2,3,4-tri-O-acetyl-.alpha.-D-glucopyranosyl bromide)uronate and sodium bicarbonate in a two-phase system of water and an org. solvent. The synthetic approach successfully yielded quaternary ammonium-linked glucuronides of 20 drugs and two of their phase I metabolites. The drugs were from various pharmacol. classes: H1 antihistamines, antipsychotic agents, and tricyclic antidepressants. Phys. data such as HPLC retention times, and diagnostic fast-atom bombardment mass spectra and <sup>1</sup>H NMR spectra were obtained. These should aid in the characterization of compds. in samples isolated from biol. media.

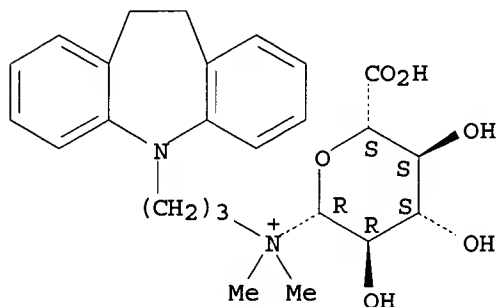
IT **86492-48-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 86492-48-0 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanaminium, N-.beta.-D-glucopyranuronosyl-10,11-dihydro-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 35 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:633659 CAPLUS

DOCUMENT NUMBER: 117:233659

TITLE: Molecular design and chemical synthesis of potent enediynes. 1. Dynemicin model systems equipped with N-tethered triggering devices

AUTHOR(S): Nicolaou, K. C.; Maligres, P.; Suzuki, T.; Wendeborn, S. V.; Dai, W. M.; Chadha, R. K.

CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA

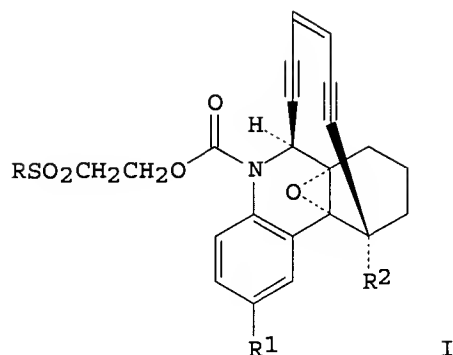
SOURCE: J. Am. Chem. Soc. (1992), 114(23), 8890-907

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB In this article the mol. design and chem. synthesis of a series of enediynes I (R = Ph, 1-naphthyl, 2-naphthyl; R1 = H, MeO, HOCH2CH2O, HOCH2C.tplbond.C; R2 = H, MeO, HOCH2CH2O) related to the dynemicin A structure and carrying N-tethered triggering devices are described. The design envisioned the [(arylsulfonyl)ethoxy]carbonyl group attached at the nitrogen atom as a triggering device for the Bergman cycloaromatization reaction because of its ability to undergo .beta.-elimination under basic conditions, liberating the labile free amine intermediate. A no. of tethering groups on the arom. ring were also installed in these systems for future incorporation of other desirable moieties such as delivery systems and soly. enhancers. Bergman cycloaromatization expts. under basic and acidic conditions demonstrated the abilities of these compds. to generate benzenoid diradicals. A no. of potent DNA-cleaving compds. and cytotoxic agents emerged from these studies.

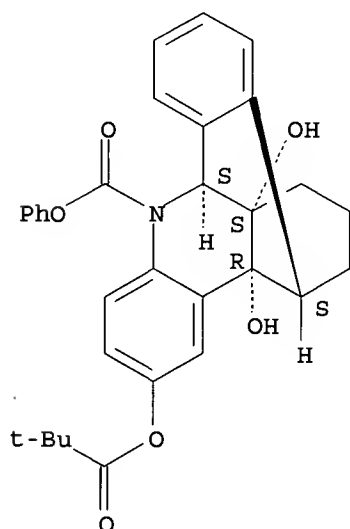
IT 144127-87-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 144127-87-7 CAPLUS

11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
2-(2,2-dimethyl-1-oxopropoxy)-11,12-dihydro-12,13-dihydroxy-, phenyl  
ester, (6.alpha.,11.alpha.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 36 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:633658 CAPLUS

DOCUMENT NUMBER: 117:233658

TITLE: Molecular design and chemical synthesis of potent enediynes. 2. Dynemicin model systems equipped with C-3 triggering devices and evidence for quinone methide formation in the mechanism of action of dynemicin A

AUTHOR(S): Nicolaou, K. C.; Dai, W. M.

CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA

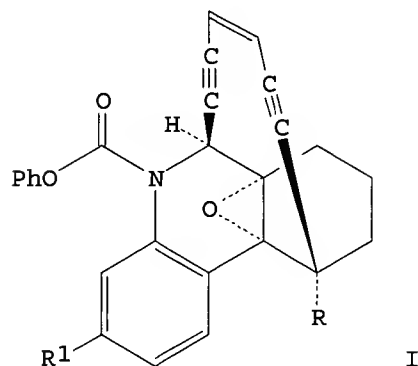
SOURCE: J. Am. Chem. Soc. (1992), 114(23), 8908-21

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Continuing the theme of the preceding article, this paper describes the synthesis and chem. properties of designed enediynes related to dynemicin A. These model systems are equipped with triggering devices at C-3 of the arom. nucleus. The design of these compds., e.g., I (R = H, R1 = Me3CCO2; R = HO, R1 = 2-O2NC6H4CH2) was based on the hypothesis that a C-3 phenolic group generated in situ would be capable of promoting epoxide opening and subsequent Bergman cycloaromatization according to the dynemicin A cascade. Exposure of I (R = H, HO; R1 = Me3CCO2) to aq. LiOH in EtOH led to Bergman cycloaromatization products. I (R = HO, AcO; R1 = 2-O2NC6H4CH2), bearing the 2-nitrobenzyl group at C-3, were photolytically converted to free phenolic systems I (R = HO, AcO; R1 = HO). Reaction of I (R = HO, AcO; R1 = HO) with the nucleophiles EtOH, EtSH, or PrNH2 under anaerobic conditions in basic buffer solns. led to aromatized products. Exposure of I (HO, MeO; R1 = HO) on the other hand, with EtOH under aerobic conditions in basic buffer solns. furnished novel quinone methide epoxide systems. The chem. of I (R = HO, AcO; R1 = HO) combined with their DNA-cleaving capabilities provides support for the quinone methide mechanism of action of dynemicin A.

IT 135106-85-3P

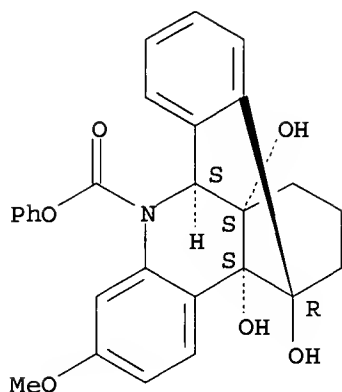
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 135106-85-3 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
11,12-dihydro-11,12,13-trihydroxy-3-methoxy-, phenyl ester,  
(6.alpha.,11.beta.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.





L4 ANSWER 37 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:613127 CAPLUS

DOCUMENT NUMBER: 117:213127

TITLE: Synthesis and photosensitized homo- and block copolymerization of a bisphenol-A derivative of dibenz[b,f]azepine

AUTHOR(S): Alimoglu, Ali K.; Bamford, Clement H.; Ledwith, Anthony; Yagci, Yusuf

CORPORATE SOURCE: Dep. Chem., Univ. Liverpool, Liverpool, L69 3BX, UK

SOURCE: Makromol. Chem. (1992), 193(6), 1551-6

CODEN: MACEAK; ISSN: 0025-116X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A bisphenol A deriv. of dibenz[b,f]azepine (I) was synthesized and characterized. Sensitized photopolymerization of I was studied in detail. The usefulness of N-acyldibenz[b,f]azepine groupings in promoting photochem. induced linking of the related mols. is further demonstrated by block copolymerization of I and polystyrene having terminal I substituents. Those reactions arise through benzophenone-sensitized photocyclodimerization of the central double bond of the moieties.

IT 144278-91-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and characterization of)

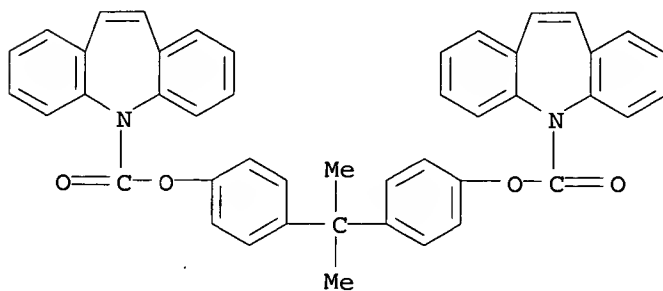
RN 144278-91-1 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxylic acid, (1-methylethylidene)di-4,1-phenylene ester, polymer with ethenylbenzene, block (9CI) (CA INDEX NAME)

CM 1

CRN 144137-97-3

CMF C45 H34 N2 O4



09/ 995,324

CM 2

CRN 100-42-5  
CMF C8 H8

$\text{H}_2\text{C}=\text{CH}-\text{Ph}$

L4 ANSWER 38 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:584282 CAPLUS

DOCUMENT NUMBER: 117:184282

TITLE: Inhibition of [3H]-MK801 binding and protection against NMDA-induced lethality in mice by a series of imipramine analogs

AUTHOR(S): McQuaid, Loretta A.; Leander, J. David; Mendelsohn, Laurane G.; Smith, Edward C. R.; Lawson, Ronald R.; Mason, Norma R.

CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, 46285, USA

SOURCE: Res. Commun. Chem. Pathol. Pharmacol. (1992), 77(2), 171-8

CODEN: RCOCB8; ISSN: 0034-5164

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of imipramine analogs were tested for inhibition of [3H]-MK801 binding and for their ability to protect against NMDA-induced lethality in mice. The structure-activity relationship (SAR) for the inhibition of [3H]-MK801 binding found primary amines on short linkers to be optimum. For protection against NMDA lethality, compds. contg. an unsatd. link to a cyclic amine were the most potent analogs tested. Possible explanations for the lack of correlation obsd. are briefly discussed.

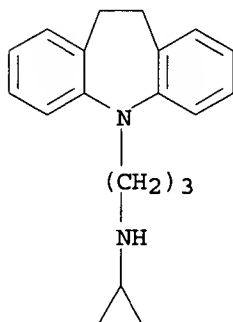
IT 143999-56-8

RL: BIOL (Biological study)

(MK-801 binding inhibition and protection against NMDA-induced lethality by, structure in relation to)

RN 143999-56-8 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanamine, N-cyclopropyl-10,11-dihydro- (9CI)  
(CA INDEX NAME)



L4 ANSWER 39 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:20843 CAPLUS

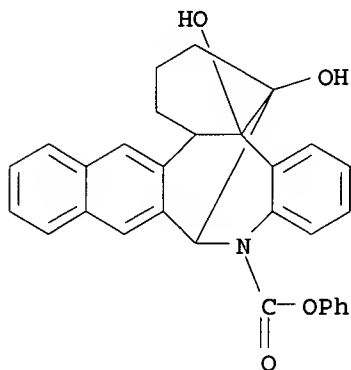
DOCUMENT NUMBER: 116:20843

TITLE: Novel enediynes equipped with triggering and detection devices. Isolation of cis-diol models of the

AUTHOR(S): dynemicin a cascade  
 Nicolaou, K. C.; Hong, Y. P.; Torisawa, Y.; Tsay, S. C.; Dai, W. M.  
 CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA  
 SOURCE: J. Am. Chem. Soc. (1991), 113(26), 9878-80  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Enedynes I (R = H, PhO<sub>2</sub>C; n = 1,2) were prepd. and studied. I (R = PhO<sub>2</sub>C; n = 1,2) were cycloaromatized to give arenes II, whereas I (R = H, n = 1,2) were cleaved to give cis-diols III. The fluorescence spectra of II, the DNA cleaving activity of I-III, and the anticancer activity of III are also reported.  
 IT **137648-63-6P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and fluorescence spectrum of)  
 RN 137648-63-6 CAPLUS  
 CN 13,6,14-[1]Butanyl[4]ylidenebenzo[b]naphth[2,3-f]azocine-5(6H)-carboxylic acid, 13,14-dihydro-14,15-dihydroxy-, phenyl ester, (6.alpha.,13.alpha.,14.beta.,15R\*)- (9CI) (CA INDEX NAME)



L4 ANSWER 40 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1991:669992 CAPLUS  
 DOCUMENT NUMBER: 115:269992  
 TITLE: Glucuronidation of imipramine in rabbit and human liver microsomes: assay conditions and interaction with other tertiary amine drugs  
 AUTHOR(S): Coughtrie, Michael W. H.; Sharp, Sheila  
 CORPORATE SOURCE: Dep. Biochem. Med., Univ. Dundee, Dundee, DD1 9SY, UK  
 SOURCE: Biochem. Pharmacol. (1991), 42(7), 1497-501  
 CODEN: BCPA6; ISSN: 0006-2952  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The glucuronidation of imipramine was studied in vitro using human and rabbit liver microsomal preps. The effects of pH, microsomal protein concn., incubation time, detergent/protein ratio, and other factors were evaluated. The inhibitor effects of 8 drugs (cyproheptadine, ketotifen, cyclizine, amitriptyline, chlorpromazine, promethazine, carbamazepine,

chlorphenizamine on the activity of imipramine UDP-glucuronosyltransferase were quantified.

IT 86492-48-0

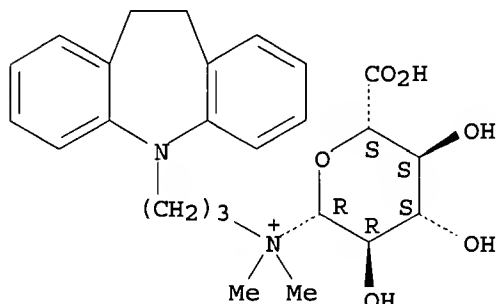
RL: FORM (Formation, nonpreparative)

(formation of, kinetics of, drugs interaction with, in liver microsomes, in human and rabbit)

RN 86492-48-0 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanaminium, N-.beta.-D-glucopyranuronosyl-10,11-dihydro-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 41 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:655858 CAPLUS

DOCUMENT NUMBER: 115:255858

TITLE: Eneidyne compounds with acid, base, and light sensitive trigger groups. Chemical simulation of dynemicin A reaction cascade

AUTHOR(S): Nicolaou, Von K. C.; Dai, W. M.; Wendeborn, S. V.; Smith, A. L.; Torisawa, Y.; Maligres, P.; Hwang, C. K.  
CORPORATE SOURCE: Dep. Chem., Res. Inst. Scripps Clin., La Jolla, CA, 92037, USA

SOURCE: Angew. Chem. (1991), 103(8), 1034-8 (See also Angew. Chem., Int. Ed. Engl., 1991, 30(8), 1032-6)  
CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal

LANGUAGE: German

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The dynemicin A model compds. I (R = H, OMe, R1 = R2 = H; R = OMe, R1 = CO2Ph, R2 = OH; R = OH, R1 = CO2Ph, R2 = OH, O2CCMe3, OMe) underwent cycloaromatization on treatment with nucleophiles with acid, base, or photochem. activation to give the benzo-bridged products II (R3 = OPh, SPh, OH, OEt, SET, NHPr). I (R = OMe, R1 = CO2Ph, R2 = OH), on the other hand, gave the dienones III (R = OMe, R1 = CO2Ph, H). III (R = OH, R1 = CO2Ph) was also formed as a byproduct from I (R = OH, R1 = CO2Ph, R2 = OH). I (R-R2 = H; R = R2 = OH, R1 = CO2Ph) and III (R = OH, R1 = CO2Ph) caused significant cleavage of .PHI.X174 DNA strands. I (R = OMe, R1 = R2 = H; R = OMe, R1 = CO2Ph, R2 = OH) and III (R = OMe, R1 = H, CO2Ph) were less active.

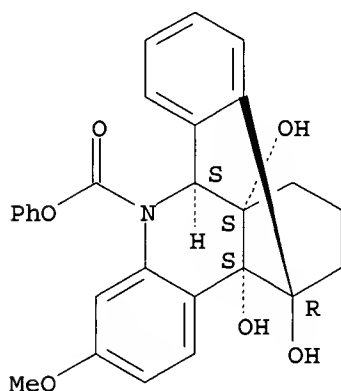
IT 135106-85-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 135106-85-3 CAPLUS

CN 11,6,12-[1]Butanyl [4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
11,12-dihydro-11,12,13-trihydroxy-3-methoxy-, phenyl ester,  
(6.alpha.,11.beta.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 42 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:247164 CAPLUS

DOCUMENT NUMBER: 114:247164

TITLE: Preparation of 3-alkoxycarbonylamino-5-aminoacyl-5H-dibenz[b,f]azepines as antiarrhythmics

INVENTOR(S): Wunderlich, Helmut; Stark, Andreas; Lohmann, Dieter;  
Zenker, Lothar; Bartsch, Reni; Poppe, Hildegard;  
Skoldinov, A. P.; Kaverina, N. V.; Grizenko, A. N.; et  
al.

PATENT ASSIGNEE(S) : VEB Arzneimittelwerk Dresden, Ger. Dem. Rep.

SOURCE: Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

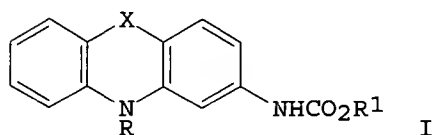
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 405255	A2	19910102	EP 1990-111337	19900615
EP 405255	A3	19910807		
R: AT, CH, DE, ES, FR, GB, IT, LI, SE				
DD 296915	A5	19911219	DD 1989-330175	19890630
JP 03038570	A2	19910219	JP 1990-169656	19900627
US 5192760	A	19930309	US 1990-546375	19900629

PRIORITY APPLN. INFO.: DD 1989-330175 19890630

OTHER SOURCE(S) :                    MARPAT 114:247164

GI



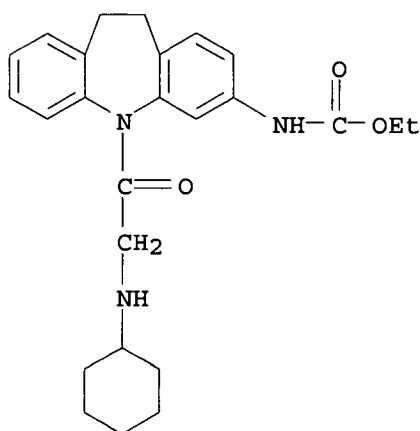
AB The title compds. [I; R = CO(CH<sub>2</sub>)<sub>n</sub>CHR<sub>2</sub>; R<sub>1</sub> = alkyl; R<sub>2</sub> = H, (cyclo)alkyl, aralkyl, CH<sub>2</sub>CH<sub>2</sub>OH; X = CH<sub>2</sub>CH<sub>2</sub>, CH:CH; n = 1-5] were prepd. Thus, I (R<sub>1</sub> = Et, X = CH<sub>2</sub>CH<sub>2</sub>) (II; R = COCH<sub>2</sub>Cl) was stirred 1 h at 60.degree. and 4 h at 70-75.degree. with aq. EtNH<sub>2</sub> in EtOH to give II (R = COCH<sub>2</sub>NH<sub>2</sub>), which had ED<sub>73</sub> of 0.09 mg/kg i.v. against aconitine-induced arrhythmias in rats.

IT **134068-22-7P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as antiarrhythmic agent)

RN 134068-22-7 CAPLUS

CN Carbamic acid, [5-[(cyclohexylamino)acetyl]-10,11-dihydro-5H-dibenz[b,f]azepin-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:246836 CAPLUS

DOCUMENT NUMBER: 114:246836

TITLE: Squaric acid diethyl ester: a new coupling reagent for the formation of drug biopolymer conjugates.

Synthesis of squaric acid ester amides and diamides  
AUTHOR(S): Tietze, Lutz F.; Arlt, Michael; Beller, Matthias; Gluesenkamp, Karl Heinz; Jaehde, Eckhard; Rajewsky, Manfred F.

CORPORATE SOURCE: Inst. Org. Chem., Univ. Goettingen, Goettingen, D-3400, Fed. Rep. Ger.

SOURCE: Chem. Ber. (1991), 124(5), 1215-21

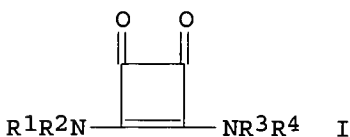
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:246836

GI



AB The amidation of di-Et squarate with amines (e.g., HOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>,

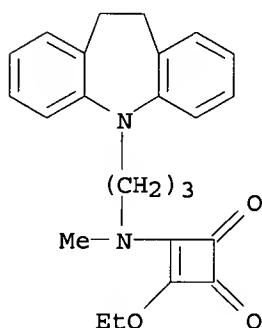
2-aminoadamantane, (+)-ephedrine, desipramine.HCl, serotonin hydrogen dioxalate, tryptamine, histamine.HCl) gave the resp. monoamides. The amidation of the latter under more basic conditions gave the resp. squaric acid diamides, e.g., I [R1 = HO(CH2)3, 2-(hydroxymethyl)-1-pyrrolidinyl, etc.; R2, R4 = H, Me; R3 = HO(CH2)3, HOCHPhCHMe, etc.]. Alc. or phenolic functions did not interfere in the coupling reactions. The reaction could be performed in buffered solns., which makes the reaction applicable to biopolymers (no data).

IT 131589-04-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 131589-04-3 CAPLUS

CN 3-Cyclobutene-1,2-dione, 3-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-4-ethoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 44 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:206847 CAPLUS

DOCUMENT NUMBER: 114:206847

TITLE: Synthesis and chemistry of dynemicin A models

AUTHOR(S): Nicolaou, K. C.; Smith, A. L.; Wendeborn, S. V.;  
Hwang, C. K.

CORPORATE SOURCE: Dep. Chem., Res. Inst. Scripps Clin., La Jolla, CA,  
92037, USA

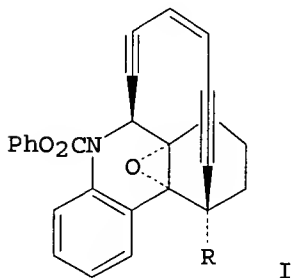
SOURCE: J. Am. Chem. Soc. (1991), 113(8), 3106-14

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis of the model systems I (R = OH, H) of dynemicin A has been achieved. These models undergo acid-induced triggering to give the corresponding Bergman-cyclized products in the presence of suitable H atom donors. Removal of the N protecting group from I (R = H) gave the

unstable free amine which caused double-stranded-DNA cleavage, presumably in a manner similar to that of dynemicin A itself. Some interesting chem. related to dicobalt complexes of the enediynes is also presented.

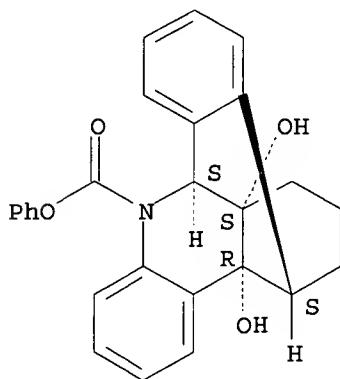
IT 130012-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 130012-98-5 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
11,12-dihydro-12,13-dihydroxy-, phenyl ester,  
(6.alpha.,11.alpha.,12.beta.,13R\*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:206399 CAPLUS

DOCUMENT NUMBER: 114:206399

TITLE: Triplet energy transfer of the intramolecular system  
having benzophenone and dibenz[b,f]azepine at the  
chain ends: chain length dependence

AUTHOR(S): Katayama, Hideaki; Maruyama, Shogo; Ito, Shinzaburo;  
Tsujii, Yoshinobu; Tsuchida, Akira; Yamamoto, Masahide

CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan

SOURCE: J. Phys. Chem. (1991), 95(9), 3480-6

CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Intramol. triplet-triplet energy transfer in a series of polymethylene chains having a benzophenone (BP) group as an energy donor and a dibenz[b,f]azepine (DBA) group as an energy acceptor [BPO(CH<sub>2</sub>)<sub>n</sub>CODBA] was studied by phosphorescence measurement and ns laser photolysis. In a rigid soln. and PMMA matrix, the quantum yield of triplet-triplet energy transfer is close to unity for chain lengths  $n < 5$ . On the basis of the through-space mechanism of energy transfer, phosphorescence-decay curves were analyzed by Dexter's equation, in which the distribution of donor-acceptor distance was calcd. by conformational-energy anal. The results of the simulation were in fairly good agreement with the exptl. obsd. decay curves. The rate const. of triplet-triplet energy transfer is strongly dependent on the chain length, i.e., about one-tenth decrease per methylene unit, and the rate is much smaller than that of singlet-singlet energy transfer.

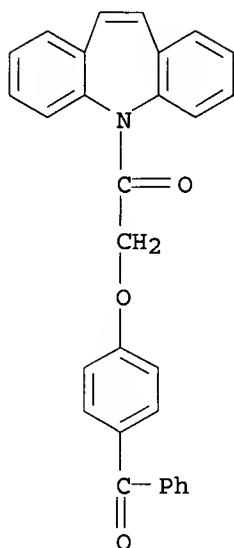
IT 133578-78-6

RL: PRP (Properties)  
(intramol. triplet-triplet energy transfer in)

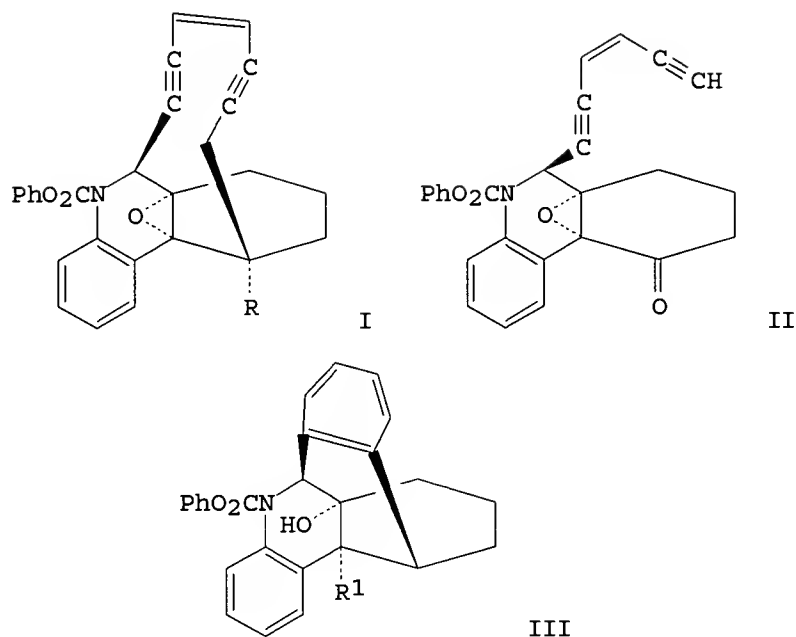
RN 133578-78-6 CAPLUS

CN 5H-Dibenz[b,f]azepine, 5-[(4-benzoylphenoxy)acetyl]- (9CI) (CA INDEX NAME)





L4 ANSWER 46 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1990:631047 CAPLUS  
 DOCUMENT NUMBER: 113:231047  
 TITLE: Synthesis of dynemicin A models  
 AUTHOR(S): Nicolaou, K. C.; Hwang, C. K.; Smith, A. L.;  
 Wendeborn, S. V.  
 CORPORATE SOURCE: Dep. Chem., Res. Inst. Scripps Clin., La Jolla, CA,  
 92037, USA  
 SOURCE: J. Am. Chem. Soc. (1990), 112(20), 7416-18  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:231047  
 GI



AB Model systems I (R = OH, H) of dynemicin A were prepd. from alkadiyne precursor II by intramol. coupling and deoxygenation of I (R = OH) to give I (R = H). The structures of I are based on spectroscopic evidence and confirmed by x-ray crystallog. anal. I (R = H) underwent Bergman-type cyclizations to benzene derivs. III (R1 = OH, Cl).

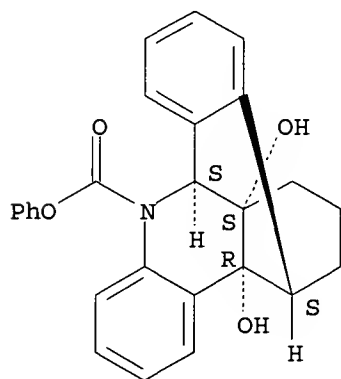
IT 130012-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 130012-98-5 CAPLUS

CN 11,6,12-[1]Butanyl[4]ylidenedibenz[b,f]azocine-5(6H)-carboxylic acid,  
11,12-dihydro-12,13-dihydroxy-, phenyl ester,  
(6.alpha.,11.alpha.,12.beta.,13R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 47 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:597753 CAPLUS

DOCUMENT NUMBER: 107:197753

TITLE: Quinone-amine reactions. Part 23. 4-Amino-1,2-

naphthoquinone derivatives of the desipramine-type psychodrugs

AUTHOR(S): Kallmayer, H. J.; Tappe, C.  
 CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes, Saarbruecken, Fed. Rep. Ger.  
 SOURCE: Pharm. Acta Helv. (1987), 62(1), 2-6  
 CODEN: PAHEAA; ISSN: 0031-6865

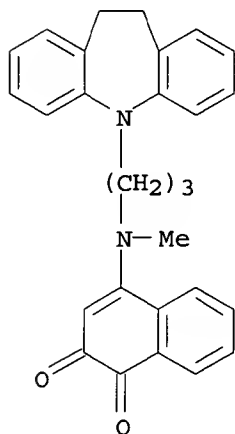
DOCUMENT TYPE: Journal  
 LANGUAGE: German

AB 1,2-Naphthoquinone-4-sulfonic acid sodium salt reacted with desipramine, nortriptyline, protriptyline, maprotiline and benzoctamine to give the corresponding 4-amino-1,2-naphthoquinones. Their spectral properties are compared with those of the corresponding isomeric 2-amino-1,4-naphthoquinones. N-Dealkylation of the 4-amino-1,2-naphthoquinone derivs. by daylight failed. Daylight does not dehydrate the nortriptylin deriv. of the 1,2-naphthoquinone unlike its 1,4-analog.

IT **111022-33-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 111022-33-4 CAPLUS

CN 1,2-Naphthalenedione, 4-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



L4 ANSWER 48 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:458823 CAPLUS

DOCUMENT NUMBER: 107:58823

TITLE: Quinone-amine reactions. Part 22: Photoreactivity from halogenated 1,4-benzoquinone derivatives of desipramine

AUTHOR(S): Kallmayer, H. J.; Tappe, Christiane  
 CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes, Saarbruecken, Fed. Rep. Ger.  
 SOURCE: Pharmazie (1986), 41(12), 832-5  
 CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal  
 LANGUAGE: German

OTHER SOURCE(S): CASREACT 107:58823

GI

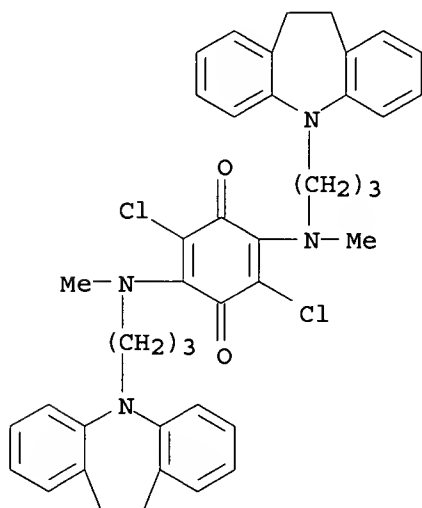
AB Treatment of chloranil with the title amine (I) gave the corresponding aminotrichloro (II) and bis(amino)dichlorobenzoquinones (III); daylight demethylates II to IV (R = Me, Q), and III under these conditions gives V (R = Me, Q). The alkyl chains are more easily lost than is the Me group. Bromanil and I gives VI, which in daylight is debrominated at C-3 to give VII.

IT 109423-34-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and photodealkylation of)

RN 109423-34-9 CAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,5-dichloro-3,6-bis[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino] - (9CI) (CA INDEX NAME)



L4 ANSWER 49 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:195991 CAPLUS

DOCUMENT NUMBER: 106:195991

TITLE: Quinone-amine reactions. Part 18:  
2-Methyl-1,4-benzoquinone derivatives from  
psychopharmacological agents with secondary amine  
structure

AUTHOR(S): Kallmayer, H. J.; Tappe, Christiane

CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes,  
Saarbruecken, D-6600, Fed. Rep. Ger.

SOURCE: Pharmazie (1986), 41(1), 29-33

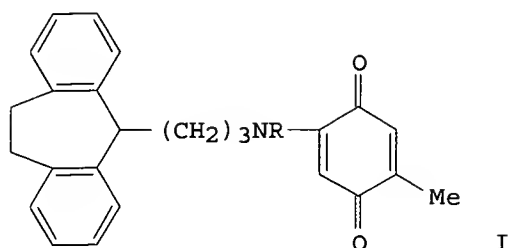
CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 106:195991

GI



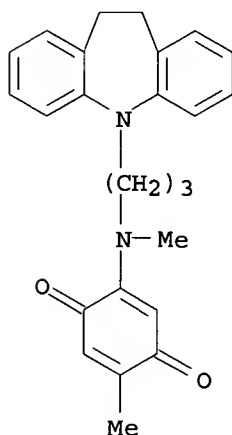
AB 2-Methyl-1,4-benzoquinone reacts with psychopharmacol. agents which are secondary amines to give red-violet aminoquinones, e.g. I (R = Me) . Daylight dealkylates the amine function from these isolated compds. to give orange-red aminoquinones, e.g. I (R = H) . Their methylamino derivs. are synthesized from 2-methyl-1,4-benzoquinone and methylamine. Mass spectra fragmentation of the aminoquinones is discussed.

IT 108141-73-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and photochem. demethylation of) .

RN 108141-73-7 CAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-5-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 50 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:138047 CAPLUS

DOCUMENT NUMBER: 106:138047

TITLE: Quinone-amine reactions. XXI. Photoreactivity of 2-amino-3-halo-1,4-naphthoquinones

AUTHOR(S): Kallmayer, Hans Joerg; Tappe, Christiane

CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes, Saarbruecken, D-6600, Fed. Rep. Ger.

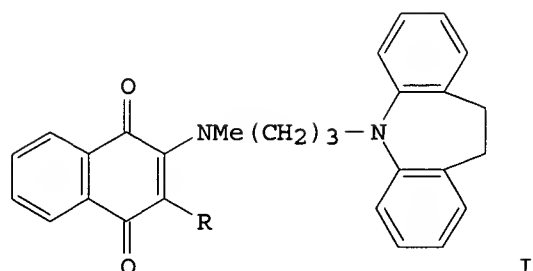
SOURCE: Arch. Pharm. (Weinheim, Ger.) (1986), 319(9), 791-8  
CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 106:138047

GI



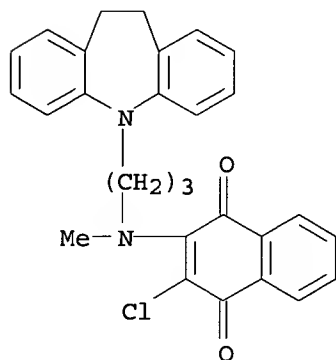
AB 2,3-Dichloro- and 2,3-dibromo-1,4-naphthoquinones react with the secondary amines desipramine, nor- and protriptyline, maprotiline, and benzoctamine to give the 2-amino-3-chloro- and 2-amino-3-bromo-1,4-naphthoquinone derivs. e.g. I (R = Cl, Br). Daylight dealkylates the amine function of chlorinated aminoquinones exclusively, whereas in the brominated aminoquinones debromination of the C-3 position neighboring the amino group is favored. The amine functions of the debrominated products are not dealkylated.

IT **107183-17-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 107183-17-5 CAPLUS

CN 1,4-Naphthalenedione, 2-chloro-3-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



L4 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:84622 CAPLUS

DOCUMENT NUMBER: 106:84622

TITLE: Tricyclic derivatives of 1,2,5-thiadiazole oxides as antihistaminics

INVENTOR(S): Gribble, Andrew Derrick; Ife, Robert John

PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK

SOURCE: Eur. Pat. Appl., 14 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 200450	A2	19861210	EP 1986-302976	19860421

EP 200450	A3	19880907		
EP 200450	B1	19900103		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 49212	E	19900115	AT 1986-302976	19860421
US 4668671	A	19870526	US 1986-854951	19860423
JP 61254585	A2	19861112	JP 1986-97812	19860425

PRIORITY APPLN. INFO.:		GB 1985-10680	19850426
		EP 1986-302976	19860421

GI For diagram(s), see printed CA Issue.

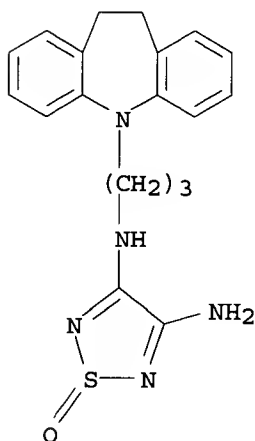
AB The title compds. I [R1 = H, C1-6 alkyl, R2CH2; R2 = (un)substituted Ph, pyridinyl; A, B = fused, (un)substituted benzo, pyrido rings; n = 2-5; m = 1, 2; X1 = O, S, R3N, CHR4, CH2CHR4, OCHR4, SCHR4; R3 = H, C1-6 alkyl, C1-6 alkanoyl; R4 = H, C1-6 alkyl] were prepd. as antihistaminics. Thus, 10H-pyrido[3,2-b][1,4]benzothiazine was N-alkylated by N-(3-bromopropyl)phthalimide, the product deprotected by hydrazinolysis, and condensed with 3,4-dimethoxy-1,2,5-thiadiazole 1-oxide and 4-(aminomethyl)pyridine to give diaminothiadiaazole II. In tests with isolated guinea pig ileum I had pA2 >7. Tablets were prepd. contg. II 55, Ca3(PO4)2.2H2O 20, microcryst. cellulose 8.0, cornstarch 8.0, polyvinylpyrrolidone 4.0, Na glycolate 4.0, Mg stearate 0.5, and coloring agent 0.5 wt. %.

IT 106561-76-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as antihistaminic)

RN 106561-76-6 CAPLUS

CN 1,2,5-Thiadiazole-3,4-diamine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-, 1-oxide (9CI) (CA INDEX NAME)



L4 ANSWER 52 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:18386 CAPLUS

DOCUMENT NUMBER: 106:18386

TITLE: Microbicidal dibenzazoles

INVENTOR(S): Fischer, Hanspeter; Buerger, Walter

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Patentschrift (Switz.), 10 pp.

CODEN: SWXXAS

DOCUMENT TYPE: Patent

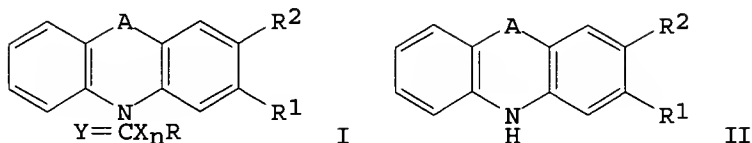
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 653675	A	19860115	CH 1983-2871	19830526

GI



AB Title compds. I [R = halo or C1-3 alkoxy (un)substituted C1-6 alkyl or C3-7 cycloalkyl; halo or Me (un)substituted C2-5 alkenyl; C3-5 alkynyl; halo, Me, or MeO (un)substituted 2-furyl; or halo, cyano, C1-3 alkyl, C1-3 alkoxy, CF<sub>3</sub>, or NO<sub>2</sub> (un)substituted Ph; n = 0, 1; X, Y = O, S; A = O, S, CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, CH:CH; R<sub>1</sub>, R<sub>2</sub> = H, halo, MeO, CF<sub>3</sub>], useful as agricultural fungicides, were prepd. by acylation of dibenzazoles II with R<sub>3</sub>Z [R<sub>3</sub> = COR, COXR; Z = a leaving group capable of N-acylation or (thio)carbonylation]. Iminodibenzyl in PhMe was treated with cyclopropylcarbonyl chloride and the mixt. refluxed 20 h to give 97% N-(cyclopropylcarbonyl)iminodibenzyl. Barley sprayed with 0.02% N-acetylminodibenzyl gave complete protection against Erysiphe graminis.

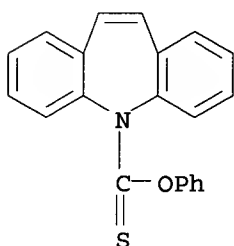
IT 105925-55-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as agricultural fungicide)

RN 105925-55-1 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carbothioic acid, O-phenyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 53 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:608588 CAPLUS

DOCUMENT NUMBER: 105:208588

TITLE: Quinone-amine reactions. XX. 1,4-Naphthoquinone derivatives of psychopharmaceutics with secondary amine structure

AUTHOR(S): Kallmayer, Hans Joerg; Tappe, Christiane

CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes, Saarbruecken, D-6600, Fed. Rep. Ger.

SOURCE: Arch. Pharm. (Weinheim, Ger.) (1986), 319(7), 607-15  
CODEN: ARPMAS; ISSN: 0365-6233

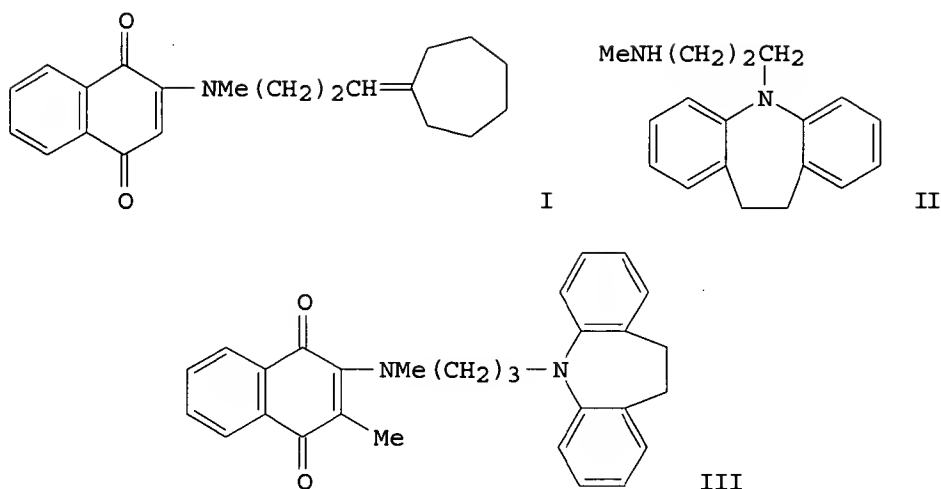
DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 105:208588

GI





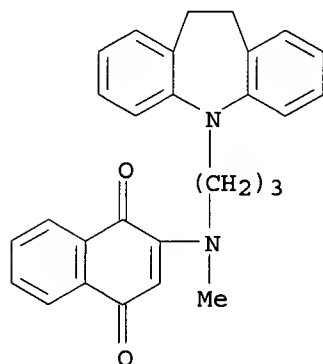
AB Desipramine-like secondary amines were treated with 1,4-naphthoquinone to yield the 2-amino-1,4-naphthoquinones, which were N-dealkylated by daylight. The nortriptyline I was dehydrogenated photochem. 2-Bromo-3-methyl-1,4-naphthoquinone and 2-methyl-2,3-epoxy-1,4-naphthoquinone were condensed with desipramine II to yield and amine III. The amine function neighboring the Me group in III produced a bathochromic effect of 44 nm.

IT 105157-96-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 105157-96-8 CAPLUS

CN 1,4-Naphthalenedione, 2-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



L4 ANSWER 54 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:460381 CAPLUS

DOCUMENT NUMBER: 105:60381

TITLE: Quinone-amine reactions. XIX: reactions between di- or trimethyl-1,4-benzoquinones and desipramine/protriptyline

AUTHOR(S): Kallmayer, Hans Joerg; Tappe, Christiane

CORPORATE SOURCE: Univ. Saarlandes, Saarbruecken, D-6600, Fed. Rep. Ger.

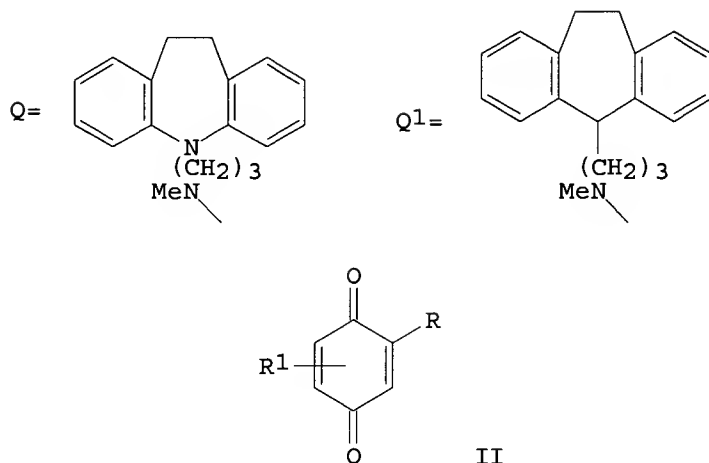
SOURCE: Arch. Pharm. (Weinheim, Ger.) (1986), 319(5), 421-7

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

09/ 995,324

LANGUAGE: German  
OTHER SOURCE(S): CASREACT 105:60381  
GI

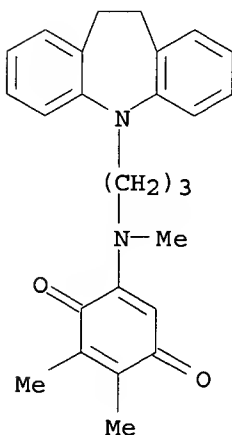


AB Desipramine (QH) (I) and Protriptyline (Q1H) react with 2,3-dimethyl-1,4-benzoquinone to yield the amino quinones II (R = Q, Q1, R1 = 5,6-Me2). II (R = Q, R1 = 3,6-Me2, 3,5-Me2, 3,5,6-Me3) are synthesized from I and 2,5- or 2,6-di- or 2,3,5-trimethyl-1,4-benzoquinones with copper(II) acetate in an oxygen atm. Daylight dealkylates the amine functions of dissolved II. Methylation at a C-5 and/or C-6 has no influence on the color of unsubstituted II (R = Q, R1 = H), but methylation adjacent to the amine function gives a bathochromic shift of 40-50 nm, independent of the substitution at C-5/6.

IT 103359-69-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

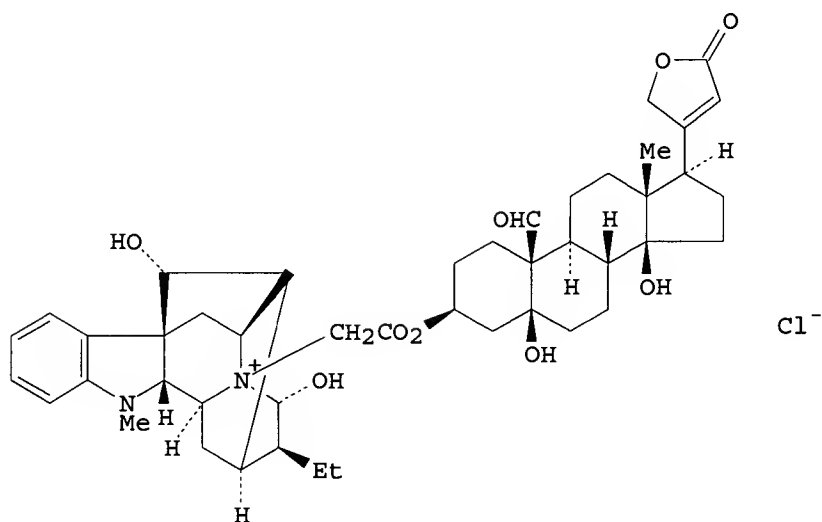
RN 103359-69-9 CAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 5-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-2,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1985:515949 CAPLUS  
DOCUMENT NUMBER: 103:115949

TITLE: Alkaloid cardenolides  
 AUTHOR(S): Makarevich, I. F.; Ivanov, L. V.; Khadzhai, Ya. I.;  
 Belokon, V. F.; Pavlova, V. V.; Klimenko, O. I.;  
 Bondar, N. I.; Uryupina, E. V.  
 CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Khim. Tekhnol. Lek.  
 Sredstv, Kharkov, USSR  
 SOURCE: Khim. Prir. Soedin. (1985), (2), 239-44  
 CODEN: KPSUAR; ISSN: 0023-1150  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB Eight alkaloid cardenolides were prepd. by previously published methods and tested for antiarrhythmic activity in rats. One of the most active of these compds., strophanthidin-3.beta.-O-acetyl-2'-N(b)ajmaline chloride (I) [83059-99-8], increased the survival rate of rats with CaCl<sub>2</sub>-induced arrhythmias from 20 to 43% when administered at 0.1 mg/kg. The i.p. LD<sub>50</sub> of I was 130 mg/kg. Two of the very active cardenolides showed even lower toxicity than I.

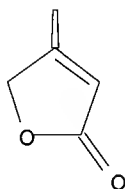
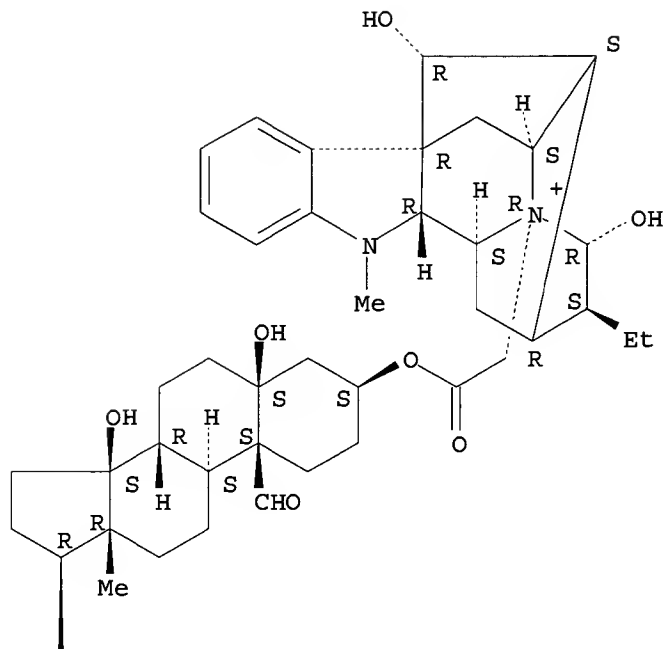
IT 67205-13-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. and antiarrhythmic activity of)

RN 67205-13-4 CAPLUS

CN Ajmalanum, 4-[2-[[[(3.beta.,5.beta.,14.beta.)-21,23-epoxy-5,14-dihydroxy-19,23-dioxo-24-norchol-20(22)-en-3-yl]oxy]-2-oxoethyl]-17,21-dihydroxy-, bromide, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● Br<sup>-</sup>

L4 ANSWER 56 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1985:419462 CAPLUS  
 DOCUMENT NUMBER: 103:19462  
 TITLE: Reporter compounds  
 INVENTOR(S): Gallop, Paul M.; Paz, Mercedes  
 PATENT ASSIGNEE(S): Children's Medical Center Corp., USA  
 SOURCE: U.S., 27 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4496722	A	19850129	US 1981-259705	19810501
US 4659817	A	19870421	US 1984-638756	19840808

09/ 995,324

PRIORITY APPLN. INFO.:

US 1980-132908

19800324

US 1981-259705

19810501

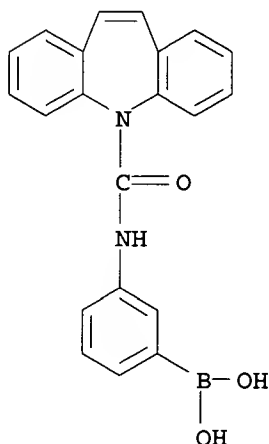
AB A new class of reagents named the Boronate-dependent Phase Transfer (BorAdept) compds. are described. They contain an org. boronic acid and one or more reporter groups, e.g., a fluorophore, a chromophore, an organometallic group, a therapeutic agent, an antigen, or an isotopically labeled group. The new compds., because of their water-soly. at or near physiol. pH, provide reporter groups with greatly enhanced versatility. Some applications of these compds. are enzymic-fluorometric detn. of glucose, staining of cells, and delivery of drugs.

IT 90393-93-4

RL: ANST (Analytical study)  
(in boronate-dependent phase transfer compds., for biochem. applications)

RN 90393-93-4 CAPLUS

CN Boronic acid, [3-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]phenyl] - (9CI)  
(CA INDEX NAME)



L4 ANSWER 57 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:220960 CAPLUS

DOCUMENT NUMBER: 102:220960

TITLE: Synthesis and synthetic utility of

1-acyl-2-alkyl-4-trimethylstannyl-1,2-dihydropyridines  
Comins, Daniel L.; Abdullah, Abdul H.; Mantlo, Nathan B.

CORPORATE SOURCE: Dep. Chem. Biochem., Utah State Univ., Logan, UT, 84322, USA

SOURCE: Tetrahedron Lett. (1984), 25(43), 4867-70

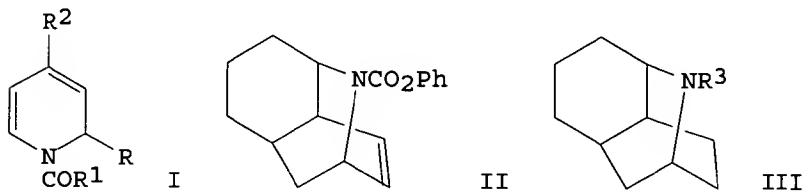
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:220960

GI

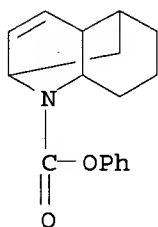


AB 4-Trimethylstannylpyridine reacted with Grignard reagents RMgCl [R = Pr, Ph, cyclohexyl, Bu, (CH<sub>2</sub>)<sub>2</sub>CH:CH<sub>2</sub>] or EtMgBr and acyl chlorides R<sub>1</sub>COC<sub>1</sub> (R<sub>1</sub> = PhO, EtO, Ph, Et, PhCH<sub>2</sub>O) to give stannyldihydropyridines I (R<sub>2</sub> = SnMe<sub>3</sub>), which were hydrolyzed with oxalic acid to give 37-70% dihydropyridines I (R<sub>2</sub> = H) overall. I [R = (CH<sub>2</sub>)<sub>3</sub>CH:CH<sub>2</sub>, R<sub>1</sub> = Ph, R<sub>2</sub> = H] cyclized to give 54% azatricycloundecene II, which was hydrogenated to form 92% azatricycloundecane III (R<sub>3</sub> = CO<sub>2</sub>Ph). Hydrolysis and N-methylation of III (R<sub>3</sub> = CO<sub>2</sub>Ph) gave 40% dihydrocannivonine (III; R<sub>3</sub> = Me).

IT **95895-25-3P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and hydrogenation of)

RN 95895-25-3 CAPLUS

CN Naphthalen-1,6-imine-9-carboxylic acid, 1,2,3,4a,5,6,8a-octahydro-, phenyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 58 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:179062 CAPLUS

DOCUMENT NUMBER: 102:179062

TITLE: Fluorescent polarization immunoassays for drugs

INVENTOR(S): Wang, Chao Huei J.; Stroupe, Stephen D.; Jolley, Michael E.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S., 4 pp. Cont.-in-part of U.S. Ser. No. 329,974.  
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4492762	A	19850108	US 1982-393577	19820630
US 4420568	A	19831213	US 1981-325872	19811130
US 5066426	A	19911119	US 1984-644172	19840823
US 4492762	B1	19910813	US 1987-90001162	19870206
US 4952691	A	19900828	US 1990-466557	19900117
US 5391740	A	19950221	US 1993-44927	19930408
PRIORITY APPLN. INFO.:			US 1980-173553	19800730
			US 1981-235259	19810217
			US 1981-325872	19811130
			US 1981-329974	19811211
			US 1981-329975	19811211
			US 1982-393577	19820630
			US 1982-443401	19821122
			US 1984-577946	19840208
			US 1986-828315	19860210
			US 1987-58638	19870603
			US 1987-90001314	19870825

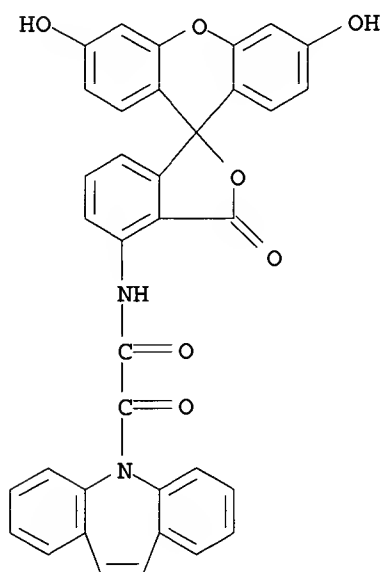
US 1988-90001614 19881005  
US 1990-465520 19900117

AB A fluorescence polarization immunoassay for detg. drugs in icteric serum or plasma is described. Thus, conducting the immunoassay in a soln. contg. effective amts. of an anionic surfactant (e.g. Na dodecyl sulfate [151-21-3], Na cholate [361-09-1], or Na toluenesulfonate [657-84-1]), to disrupt the fluorescent bilirubin-serum albumin complex in the sample, reduces the background fluorescence of the blood sample.

IT **96053-95-1P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, for fluorescence polarization immunoassay)

RN 96053-95-1 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-acetamide, N-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-4-yl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:166596 CAPLUS

DOCUMENT NUMBER: 102:166596

TITLE: The synthesis of spin-labeled imipramine analogs

AUTHOR(S): Kikelj, D.; Pecar, S.; Debeljak, B.; Karba, D.; Krbavcic, A.

CORPORATE SOURCE: Dep. Pharm., Univ. E. Kardelj, Ljubljana, 61000, Yugoslavia

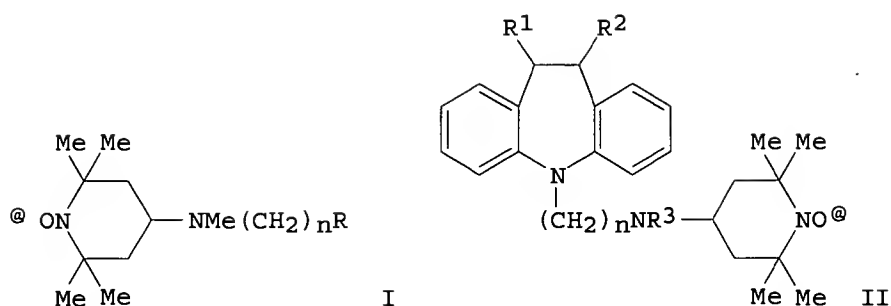
SOURCE: Synth. Commun. (1984), 14(6), 547-56  
CODEN: SYNCAV; ISSN: 0039-7911

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:166596

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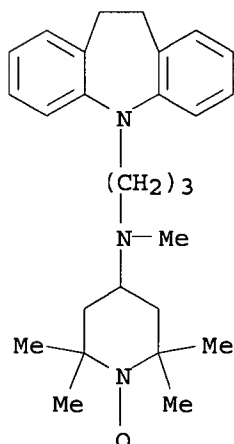
AB The spin-label piperidines I ( $R = OH$ ;  $n = 2, 3$ ) was chlorinated with 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>Cl to give I ( $R = Cl$ ), and I ( $R = OH$ ,  $n = 6$ ) was mesylated to give I ( $R = O_3SMe$ ). I ( $R = Cl$ ,  $n = 2, 3$ ;  $R = O_3SMe$ ,  $n = 6$ ) reacted with 5-H-dibenz[b,f]azepine or its 10,11-dihydro analog to give N-alkylated dibenzazepines II ( $R_1 = R_3 = H$ ;  $R_1R_2 = \text{bond}$ ;  $R_3 = Me$ ;  $n = 2, 3, 6$ ), which were treated with BrCN to give II ( $R_3 = \text{cyano}$ ). Hydrolysis or methanolysis of II ( $R_1 = R_2 = H$ ;  $R_3 = \text{cyano}$ ;  $n = 2, 3$ ) gave II [ $R_3 = CONH_2$ ,  $C(OMe):NH$ ] resp.

IT 93553-86-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyanation of)

RN 93553-86-7 CAPLUS

CN 1-Piperidinyloxy, 4-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 60 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:591486 CAPLUS

DOCUMENT NUMBER: 101:191486

TITLE: Chirospecific syntheses of (+)- and (-)-anatoxin a

AUTHOR(S): Petersen, John S.; Fels, Gregor; Rapoport, Henry

CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA

SOURCE: J. Am. Chem. Soc. (1984), 106(16), 4539-47

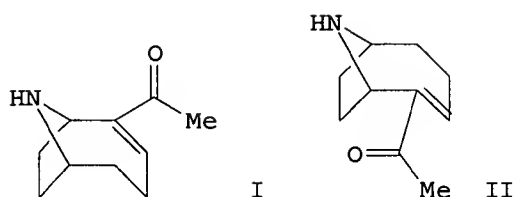
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI





AB The title compds. (I and II, resp.) of high optical purity were synthesized directly from D- and L-glutamic acid, resp. Initial carbon-carbon bond formation proceeding from the pyroglutamate via sulfide contraction and transfer of the amino acid chirality by catalytic hydrogenation are central to the synthesis. Cyclization to the bicyclic system was effected by nucleophilic attack on the iminium ion, generated by decarbonylation of the .alpha.-amino acid. The dihydroanatoxin thus formed, whose .alpha. and .beta. diastereomers were both characterized, was ultimately converted to the enone by dehydrogenation with palladium acetate.

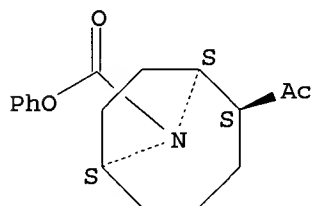
IT 90741-48-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and dehydration of)

RN 90741-48-3 CAPLUS

CN 9-Azabicyclo[4.2.1]nonane-9-carboxylic acid, 2-acetyl-, phenyl ester,  
(1S-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 61 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:420209 CAPLUS

DOCUMENT NUMBER: 101:20209

TITLE: Reporter compounds

INVENTOR(S): Gallop, Paul M.; Paz, Mercedes

PATENT ASSIGNEE(S): Children's Hospital Medical Center, USA

SOURCE: PCT Int. Appl., 109 pp.

CODEN: PIXXD2

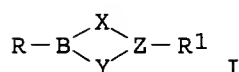
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8304255	A1	19831208	WO 1982-US725	19820526
W: DE, GB, JP				
RW: AT, BE, CH, DE, FR, GB, LU, NL, SE				
EP 110879	A1	19840620	EP 1982-902137	19820526
R: AT, BE, CH, DE, FR, GB, LI, LU, NL, SE				
PRIORITY APPLN. INFO.:			WO 1982-US725	19820526
GI				



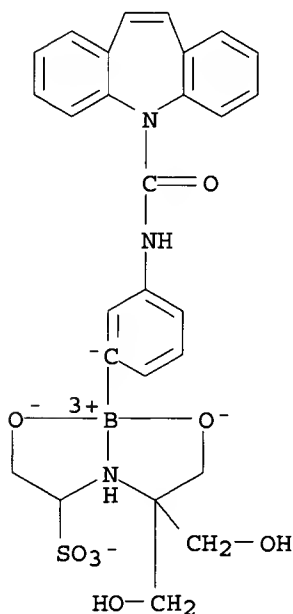
AB A new class of water-sol. reagents named boronate-dependent phase-transfer compds. (I, R = a reporter group, e.g. a fluorophore, chromophore, organometallic group, drug, antigen, or isotopically labeled group; Z = a receptor group; R<sup>1</sup> = a carrier group; and X = Y = N, O, or S) is described. I allows groups that can report on conditions within living cells or modify metabolic parameters within tissues to be taken up by the cells under nontoxic conditions. I has a broad range of applications and can be used for staining living cells for disease diagnosis, for solubilization of drugs, for staining proteins, for staining or brightening fabrics, for staining paper products, and for various assay methods, such as peroxide, antibody, glucose, and esterase detns. in which fluorescence or color intensity is measured. An app. is also described for assaying, in aq. soln., a compd. which participates in a chem. reaction which results in the prodn. of peroxide.

IT 90384-72-8

RL: ANST (Analytical study)  
(for biochem. and industrial applications)

RN 90384-72-8 CAPLUS

CN Borate(1-), [3-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]phenyl][2-hydroxy-1-[[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]amino]ethanesulfonato(3-)]-, (T-4) - (9CI) (CA INDEX NAME)



L4 ANSWER 62 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:206160 CAPLUS

DOCUMENT NUMBER: 100:206160

TITLE: Fluorescent polarization immunoassay utilizing substituted triazinylaminofluoresceins

INVENTOR(S): Wang, Chao Huei J.; Stroupe, Stephen D.; Jolley, Michael E.

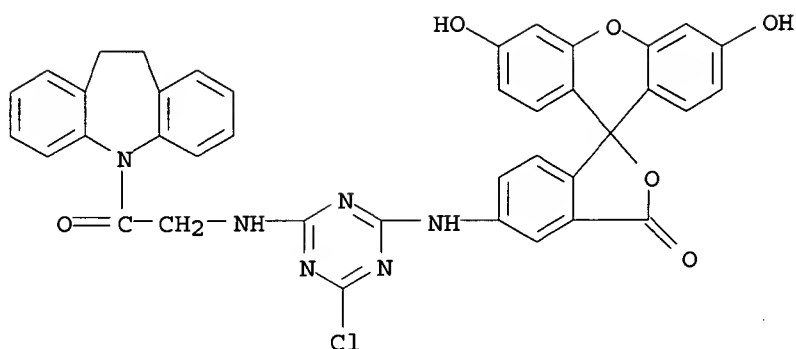
PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S., 3,553, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 6  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4420568	A	19831213	US 1981-325872	19811130
CA 1160626	A1	19840117	CA 1981-379747	19810615
GB 2081257	A	19820217	GB 1981-18754	19810618
GB 2081257	B2	19841107		
AU 8172036	A1	19820204	AU 1981-72036	19810622
AU 554360	B2	19860821		
SE 8104227	A	19820131	SE 1981-4227	19810707
DE 3129705	A1	19820527	DE 1981-3129705	19810728
DE 3129705	C2	19880310		
BE 889788	A1	19820129	BE 1981-205525	19810729
JP 57058695	A2	19820408	JP 1981-118573	19810730
US 4492762	A	19850108	US 1982-393577	19820630
US 4593089	A	19860603	US 1983-546778	19831031
US 4420568	B1	19851217	US 1984-90000617	19840824
US 4492762	B1	19910813	US 1987-90001162	19870206
US 5097097	A	19920317	US 1989-376190	19890630
PRIORITY APPLN. INFO.:			US 1980-173553	19800730
			US 1981-235259	19810217
			US 1981-325872	19811130
			US 1981-329974	19811211
			US 1981-329975	19811211
			US 1982-393577	19820630
			US 1983-546778	19831031
			US 1986-865992	19860522
			US 1987-90001314	19870825
			US 1988-90001614	19881005
AB	A fluorescent polarization immunoassay and reagents are described for the detn. of ligands (e.g., steroids, hormones, anticonvulsants, antibiotics, etc.) in biol. fluids. The reagent consists of a biol. acceptable salt (e.g., Na salt) of a triazinylaminofluorescein deriv. with an attached ligand analog and a halo or lower alkyl analog. Thus, a reagent was prepd. by reacting gentamicin sulfate (in water, pH 9.0) with 5-[(4,6-dichlorotriazin-2-yl)-amino]fluorescein (in MeOH) and the product was purified by DEAE-cellulose chromatog. The reagent was used for the detn. of gentamicin in human serum or other biol. fluids.			
IT	<b>90275-50-6P</b>			
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)			
RN	90275-50-6 CAPLUS			
CN	5H-Dibenz[b,f]azepine, 5-[[[4-chloro-6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]-1,3,5-triazin-2-yl]amino]acetyl]-10,11-dihydro- (9CI) (CA INDEX NAME)			



L4 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:558205 CAPLUS

DOCUMENT NUMBER: 99:158205

TITLE: Intramolecular Diels-Alder reactions of 2-alkenyl-1,2-dihydropyridines. An approach to the synthesis of the cis-decahydroquinoline ring system  
 AUTHOR(S): Comins, Daniel L.; Abdullah, Abdul H.; Smith, Roy K.  
 CORPORATE SOURCE: Dep. Chem. Biochem., Utah State Univ., Logan, UT, 84322, USA

SOURCE: Tetrahedron Lett. (1983), 24(27), 2711-14

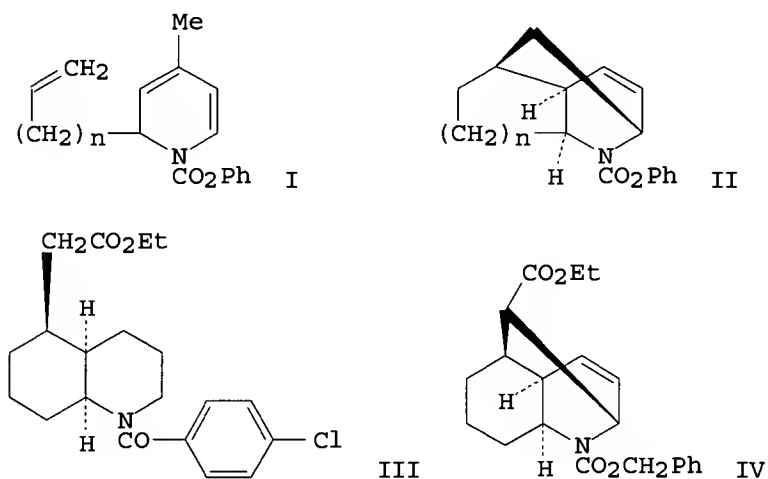
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:158205

GI



AB In refluxing decalin alkenyldihydropyridines I ( $n = 1, 2$ ) undergo an intramol. Diels-Alder reaction to give novel polycyclic compds. II. cis-Decahydroquinoline ring system III was prepd. from Diels-Alder product IV by a ring-opening reverse Mannich reaction.

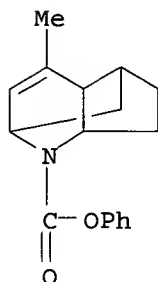
IT 87288-08-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 87288-08-2 CAPLUS

CN 1H-Inden-1,5-imine-8-carboxylic acid, 2,3,3a,4,5,7a-hexahydro-7-methyl-, phenyl ester, (1.alpha.,3a.beta.,5.alpha.,7a.beta.)- (9CI) (CA INDEX

NAME)



L4 ANSWER 64 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1983:554812 CAPLUS  
 DOCUMENT NUMBER: 99:154812  
 TITLE: Fluorescein derivatives and fluorescence polarization  
 immunoassay methods  
 INVENTOR(S): Wang, Chao Huei Jeffrey; Stroupe, Stephen Denham;  
 Jolley, Michael Ernest  
 PATENT ASSIGNEE(S): Abbott Laboratories, USA  
 SOURCE: Ger. Offen., 53 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 6  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3245854	A1	19830623	DE 1982-3245854	19821210
DE 3245854	C2	19961114		
CA 1248086	A1	19890103	CA 1982-416022	19821119
GB 2111491	A1	19830706	GB 1982-33403	19821123
GB 2111491	B2	19850821		
AU 8290880	A1	19830616	AU 1982-90880	19821125
AU 558800	B2	19870212		
FR 2518096	A1	19830617	FR 1982-20591	19821208
FR 2518096	B1	19851206		
BE 895300	A1	19830609	BE 1982-209695	19821209
JP 58113189	A2	19830705	JP 1982-214749	19821209
US 4585862	A	19860429	US 1984-577946	19840208
US 4952691	A	19900828	US 1990-466557	19900117
US 5391740	A	19950221	US 1993-44927	19930408
PRIORITY APPLN. INFO.:			US 1981-329975	19811211
			US 1984-577946	19840208
			US 1986-828315	19860210
			US 1987-58638	19870603
			US 1990-465520	19900117

AB Aminofluorescein derivs. are described as reagents for ligand detns. in biol. fluids such as serum, plasma, cerebrospinal fluid, amniotic fluid, and urine. The title method combines the specificity of immunoassays with the speed and suitability of the fluorescence polarization method. For example, lidocaine was detd. with a sulfonylidocaine - aminofluorescein conjugate and antibody to lidocaine with fluorescence polarization measurement. Polarization decreased with lidocaine concn. from 0 to 10.0 .mu.g/mL. Preps. of other conjugates are described as well as assays for carbamazepine and phenobarbital.

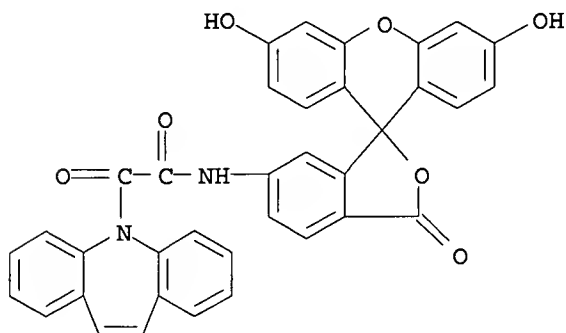
IT 87179-54-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, for fluorescence polarization immunoassay)

RN 87179-54-2 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-acetamide, N-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 65 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:447488 CAPLUS

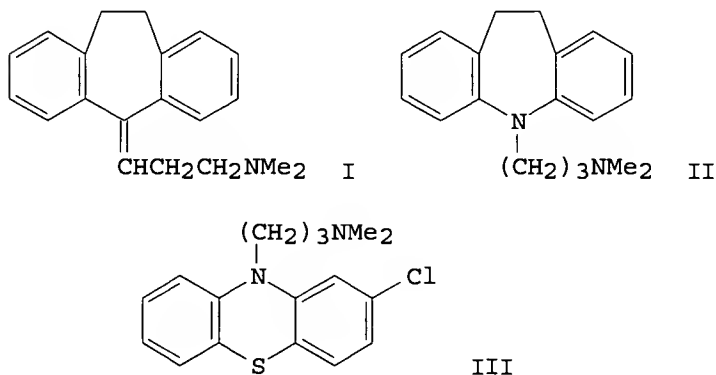
DOCUMENT NUMBER: 99:47488

TITLE: Quaternary ammonium-linked glucuronides of amitriptyline, imipramine, and chlorpromazine  
 AUTHOR(S): Lehman, James P.; Fenselau, Catherine; Depaulo, J. R.  
 CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA

SOURCE: Drug Metab. Dispos. (1983), 11(3), 221-5  
 CODEN: DMDSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal  
 LANGUAGE: English

GI



AB The quaternary ammonium-linked glucuronides of amitriptyline (I) [86492-47-9], imipramine (II) [86492-48-0] and chlorpromazine (III) [86492-49-1] were shown to be conjugated in vitro using an immobilized rabbit hepatic microsomal enzyme prepn. Fast atom bombardment mass spectrometry could be used for direct characterization of these involatile, thermally labile metabolites. The quaternary ammonium-linked glucuronides of amitriptyline and imipramine were present in urine from patients receiving therapeutic doses of these tricyclic antidepressants.

IT 86492-48-0

RL: BIOL (Biological study)

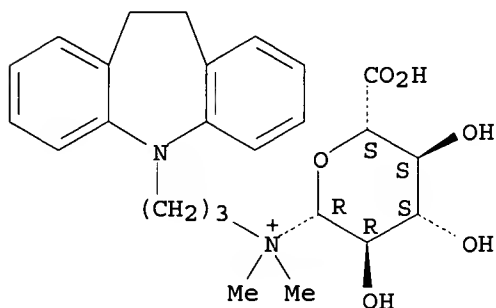
09/ 995,324

(as imipramine metabolite, in humans and lab. animals)

RN 86492-48-0 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanaminium, N-.beta.-D-glucopyranuronosyl-10,11-dihydro-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:563430 CAPLUS

DOCUMENT NUMBER: 97:163430

TITLE: N6-Substituted adenosines

INVENTOR(S): Henderson, Richard E. L.; Malek, Nancy J.; Moormann, Alan E.; Pitzele, Barnett S.

PATENT ASSIGNEE(S): Searle, G. D., and Co., USA

SOURCE: U.S., 5 pp. Cont.-in-part of U.S. Ser. No. 157,625, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4340730	A	19820720	US 1981-229824	19810130
AU 8171399	A1	19811217	AU 1981-71399	19810605
NL 8102745	A	19820104	NL 1981-2745	19810605
GB 2077725	A	19811223	GB 1981-17521	19810608
ES 502851	A1	19820401	ES 1981-502851	19810608
BE 889137	A1	19811209	BE 1981-205033	19810609
DK 8102512	A	19811210	DK 1981-2512	19810609
SE 8103580	A	19811210	SE 1981-3580	19810609
FR 2483929	A1	19811211	FR 1981-11331	19810609
DE 3122784	A1	19820506	DE 1981-3122784	19810609
JP 57130997	A2	19820813	JP 1981-88763	19810609

PRIORITY APPLN. INFO.:

US 1980-157625

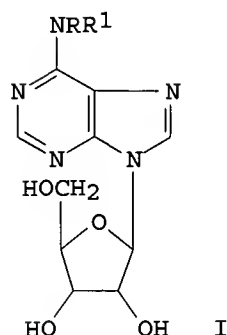
US 1981-229824

19800609

19810130

OTHER SOURCE(S): CASREACT 97:163430

GI



AB Adenosines I [R = H, C1-6 alkyl; R1 = p-Me2NC6H4CH2CH2, (CH2)<sub>n</sub>CO2R2 (n = 3-11, R2 = H, C1-20 alkyl), 3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl; or NRR1 = 4-substituted 1-piperazinyl], useful as antihypertensives (no data), were prepd. Thus, a mixt. of 15.0 g 6-chloropurine riboside, 15.2 g H2N(CH2)4CO2H, 11.1 g Bu3N in 90% aq. PROH was refluxed for 2 days to give 12.9 g I [R = H, R1 = (CH2)4CO2H].

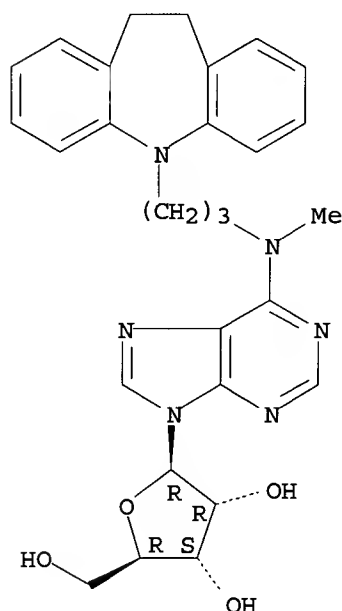
IT **81893-83-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 81893-83-6 CAPLUS

CN Adenosine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 67 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:545128 CAPLUS

DOCUMENT NUMBER: 97:145128

TITLE: Transformed cardiac glycosides and aglycones with improved therapeutic properties

AUTHOR(S): Makarevich, I. F.

CORPORATE SOURCE: Chem.-Pharm. Res. Inst., Kharkov, 310085, USSR



SOURCE: Int. Conf. Chem. Biotechnol. Biol. Act. Nat. Prod.,  
[Proc.], 1st (1981), Volume 3, Issue 2, 146-9.  
Editor(s): Atanasova, B. Bulg. Acad. Sci.: Sofia,  
Bulg.  
CODEN: 47YUAB

DOCUMENT TYPE: Conference

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Cardenolides and bufadienolides I-III (R = Me, CHO; R1 = H, HO; X = Cl, Br) of ajmaline were prepd. and their mol. structure detd. by IR spectroscopy. I-III relieve cardiac arrhythmia and tonicize cardiac activity without decreasing blood pressure, and are less toxic than simple mixts. of ajmaline and cardiac aglycons.

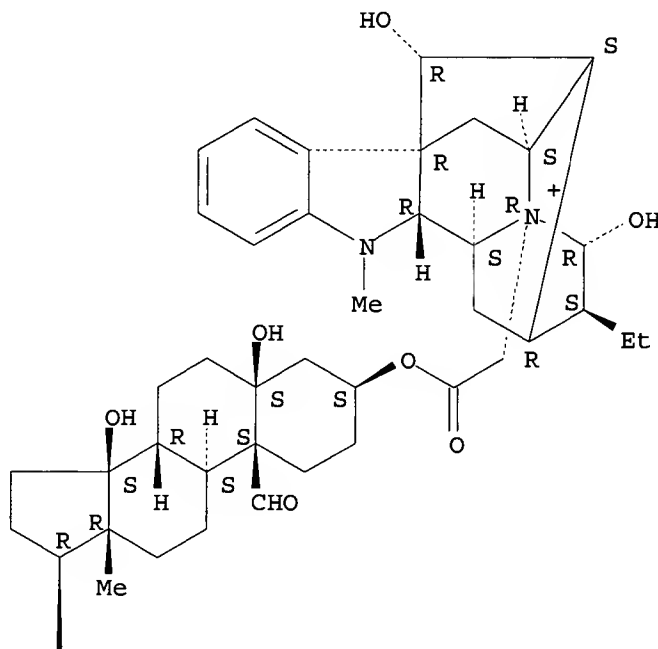
IT **67205-13-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and antiarrhythmia activity of)

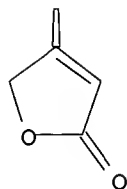
RN 67205-13-4 CAPLUS

CN Ajmalanum, 4-[2-[[[(3.beta.,5.beta.,14.beta.)-21,23-epoxy-5,14-dihydroxy-19,23-dioxo-24-norchol-20(22)-en-3-yl]oxy]-2-oxoethyl]-17,21-dihydroxy-, bromide, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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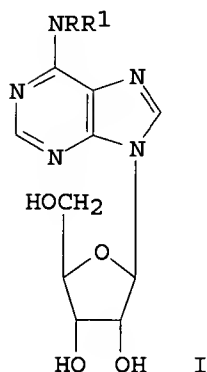


● Br<sup>-</sup>

L4 ANSWER 68 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1982:218195 CAPLUS  
 DOCUMENT NUMBER: 96:218195  
 TITLE: N6-Substituted adenosines used as antihypertension medicines, therapeutic compositions and pharmaceutical forms containing them  
 INVENTOR(S): Henderson, Richard Elliot Lee; Malek, Nancy Joan; Morrman, Alan Edward; Pitzele, Barnett Sylvain  
 PATENT ASSIGNEE(S): Searle, G. D., and Co., USA  
 SOURCE: Fr. Demande, 15 pp.  
 CODEN: FRXXBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2483929	A1	19811211	FR 1981-11331	19810609
US 4340730	A	19820720	US 1981-229824	19810130
PRIORITY APPLN. INFO.:			US 1980-157625	19800609
			US 1981-229824	19810130

GI



AB Adenosines I [R = H; C1-6 alkyl; R1 = H, 4-methyl-5-[(2-aminoethyl)thiomethyl]imidazolyl, 2-(heptamethyleniminyl)ethyl, 4-(Me2N)C6H4(CH2)2, 3-(10,11-dihydro-5H-dibenzo[b,f]azepin-5-yl)propyl, (CH2)nCO2R2 (R2 = H, C1-20 alkyl, n = 3-11); or NRR1 = substituted piperazinyl], useful as antihypertensives (no data), were prepd. Thus, 15.0 g 6-chloropurine riboside was refluxed with 15.2 g H2N(CH2)4CO2H in

09/ 995,324

90% aq. propanol in the presence of Bu<sub>3</sub>N to give 12.9 g I [R = H, R<sub>1</sub> = (CH<sub>2</sub>)<sub>4</sub>CO<sub>2</sub>H].

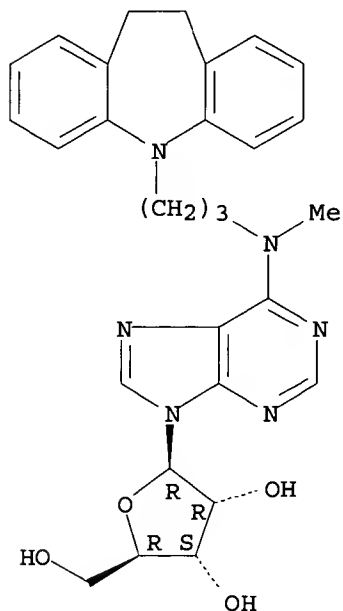
IT 81893-83-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 81893-83-6 CAPLUS

CN Adenosine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:68789 CAPLUS

DOCUMENT NUMBER: 96:68789

TITLE: Quinone-amine reactions. V: Color products of  
quinhydrone/desipramine reaction

AUTHOR(S): Kallmayer, Hans Joerg; Tappe, Christiane

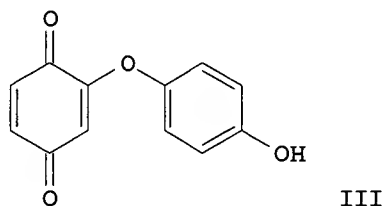
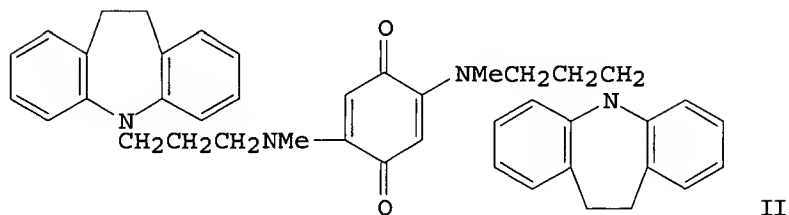
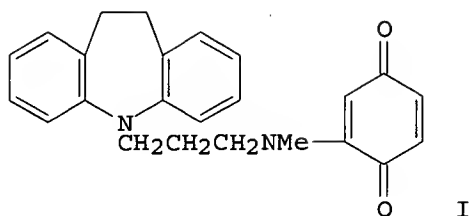
CORPORATE SOURCE: Fachrichtung Pharm. Chem., Univ. Saarlandes,  
Saarbruecken, 6600, Fed. Rep. Ger.

SOURCE: Arch. Pharm. (Weinheim, Ger.) (1981), 314(10), 884-8  
CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



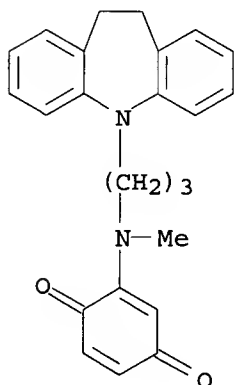
AB 1,4-Benzoquinone reacted with desipramine in CH<sub>2</sub>Cl<sub>2</sub> to give 60% intense red [(dibenzazepinylpropyl)amino]benzoquinone I and weakly colored bis compd. II. The formation of phenoxybenzoquinones, e.g. III, was not obsd.

IT 80596-46-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, with desipramine)

RN 80596-46-9 CAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



L4 ANSWER 70 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:545614 CAPLUS

DOCUMENT NUMBER: 93:145614

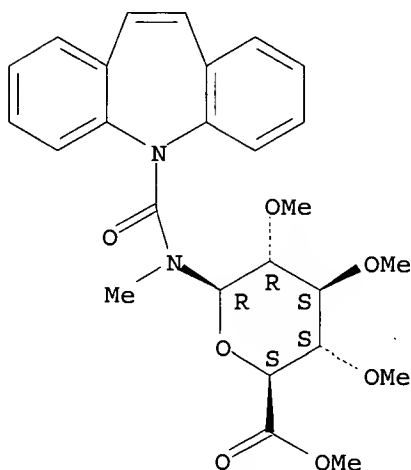
TITLE: Analysis of intact glucuronides by mass spectrometry and gas chromatography-mass spectrometry. A review

AUTHOR(S): Fenselau, Catherine; Johnson, Leslie P.

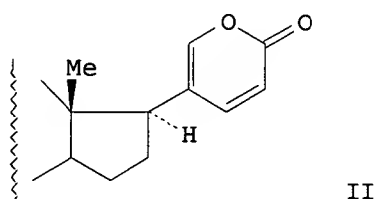
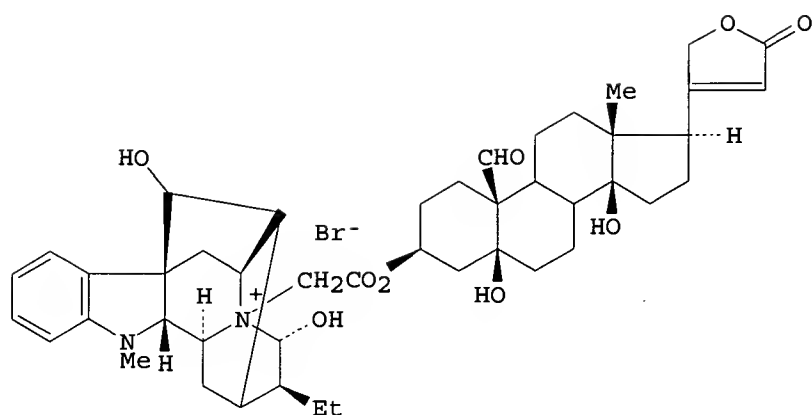
09/ 995,324

CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA  
SOURCE: Drug Metab. Dispos. (1980), 8(4), 274-83  
CODEN: DMDSAI; ISSN: 0090-9556  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English  
AB A review with 129 refs.  
IT 75041-37-1  
RL: PRP (Properties)  
(mass spectrum of)  
RN 75041-37-1 CAPLUS  
CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)methylamino]-2,3,4-tri-O-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1980:129153 CAPLUS  
DOCUMENT NUMBER: 92:129153  
TITLE: Cardenolide and bufadienolide derivatives of ajmaline  
AUTHOR(S): Makarevich, I. F.; Khadzhai, Ya. I.; Nikolaeva, A. V.; Pavlova, V. V.  
CORPORATE SOURCE: Khar'k. Nauchno-Issled. Khim.-Farm. Inst., Kharkov, USSR  
SOURCE: Khim. Prir. Soedin. (1979), (4), 537-40  
CODEN: KPSUAR; ISSN: 0023-1150  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI



AB Title compds. I and II were prepd. by condensation of ajmaline with 3-O-(bromoacetyl)strophanthidin and 3-O-(bromoacetyl)hellebrigenin. Antiarrhythmic activity of I was not accompanied by an increase in blood pressure.

IT **67205-13-4P**

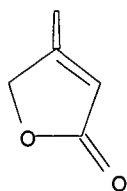
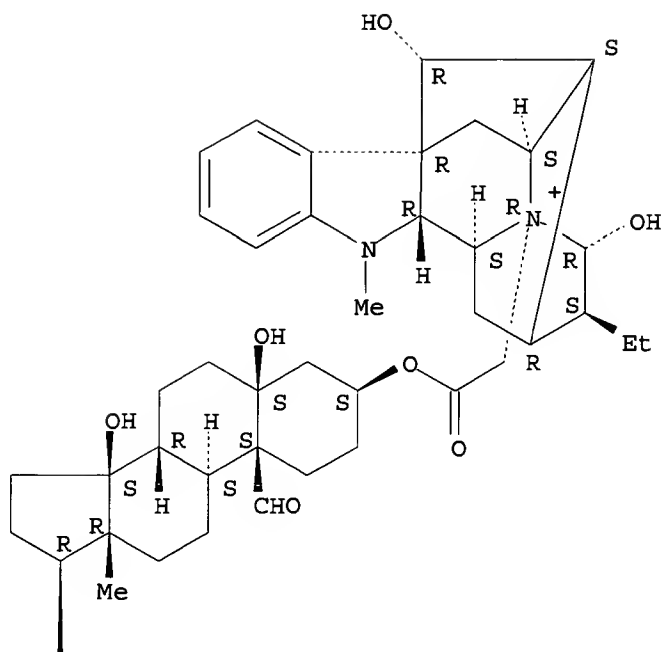
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and antiarrhythmic activity of)

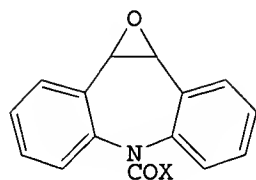
RN 67205-13-4 CAPLUS

CN Ajmalanum, 4-[2-[[[(3.beta.,5.beta.,14.beta.)-21,23-epoxy-5,14-dihydroxy-19,23-dioxo-24-norchol-20(22)-en-3-yl]oxy]-2-oxoethyl]-17,21-dihydroxy-, bromide, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 72 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1979:115115 CAPLUS  
 DOCUMENT NUMBER: 90:115115  
 TITLE: Synthesis and pharmacology of  
 dibenz[b,f]oxiren[d]azepine derivatives  
 AUTHOR(S): Kawashima, Kenya; Ishiguro, Toshihiro; Chiba,  
 Sukehiro; Nagawa, Yuji  
 CORPORATE SOURCE: Takeda Res. Lab., Osaka, Japan  
 SOURCE: Takeda Kenkyusho Ho (1978), 37(1-2), 12-20  
 CODEN: TAKHAA; ISSN: 0371-5167  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I, X=H, halo, amino

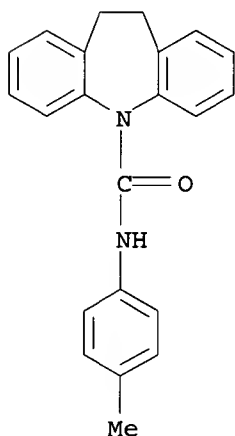
AB 1A,10b-dihydro-6H-dibenz[b,f]oxiren[d]azepines (I) were synthesized by epoxidn. of 5H-dibenz[b,f]azepines with org. peracids. The carbamoyl deriv. (I, X = NH<sub>2</sub>) [36507-30-9] showed more potent anticonvulsant activity than the ref. drug, carbamazepine, while the acute toxicity was comparable.

IT 69477-21-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 69477-21-0 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-N-(4-methylphenyl)-  
(9CI) (CA INDEX NAME)



L4 ANSWER 73 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1979:12377 CAPLUS

DOCUMENT NUMBER: 90:12377

TITLE: Analysis of psychopharmaceuticals: lofepramine  
(Gamonil)

AUTHOR(S): Elden, Fritz; Schmiz, Elisabeth

CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Muenchen,  
Munich, Ger.

SOURCE: Pharm. Ztg. (1978), 123(41), 1796-801

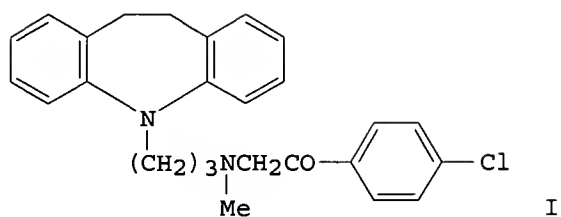
CODEN: PHZIAP; ISSN: 0031-7136

DOCUMENT TYPE: Journal

LANGUAGE: German

GI





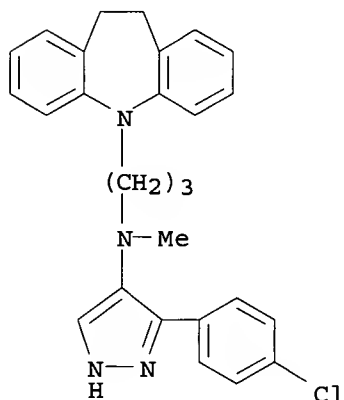
AB Thin-layer chromatog., UV, IR and NMR spectra for Gamonil (lofepramine) (I) [23047-25-8], I-HCl [26786-32-3] and prepn. of I derivs. for anal. are described. NMR spectra data and thin-layer chromatog. Rf values for several related dibenzazepine and dibenzocycloheptene derivs. are also given.

IT 68671-39-6P

RL: PREP (Preparation)  
(prepn. of, for lofepramine anal.)

RN 68671-39-6 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-propanamine, N-[3-(4-chlorophenyl)-1H-pyrazol-4-yl]-10,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 74 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:590725 CAPLUS

DOCUMENT NUMBER: 89:190725

TITLE: Newer aspects of the biotransformation of carbamazepine: structural characterization of highly polar metabolites

AUTHOR(S): Richter, W. J.; Kriemler, P.; Faigle, J. W.

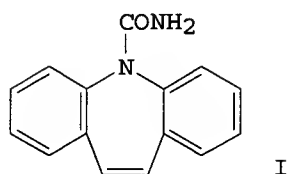
CORPORATE SOURCE: Pharm. Div., Ciba-Geigy, Basel, Switz.

SOURCE: Recent Dev. Mass Spectrom. Biochem. Med., [Proc. Int. Symp.], 4th (1978), Meeting Date 1977, Volume 1, 1-14.  
Editor(s): Frigerio, Alberto. Plenum: New York, N. Y.  
CODEN: 38XPAL

DOCUMENT TYPE: Conference

LANGUAGE: English

GI



AB The biotransformation of carbamazepine (I) [298-46-4] by man was followed by examg. the urine for metabolites. The I metabolites were isolated by a variety of chromatog. procedures, and structures of the metabolites or their derivs. were ascertained by field desorption and electron impact mass spectroscopy. Most I metabolites were products of oxidn. of the arom. ring, but other metabolites, unchanged I, and the N-glucuronide of I [60342-79-2] were also detected in urine.

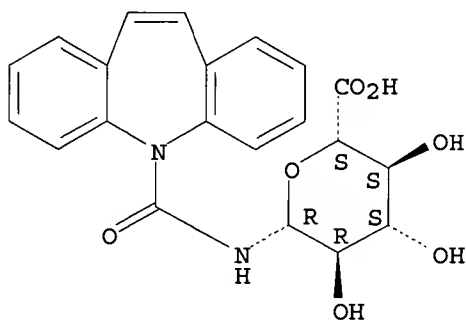
IT 60342-79-2

RL: BIOL (Biological study)  
(as carbamazepine metabolite)

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 75 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:590664 CAPLUS

DOCUMENT NUMBER: 89:190664

TITLE: Characterization of glucuronide metabolites of carbamazepine in human urine by gas chromatography and mass spectrometry

AUTHOR(S): Lynn, R. K.; Smith, R. G.; Thompson, R. M.; Deinzer, M. L.; Griffin, D.; Gerber, N.

CORPORATE SOURCE: Med. Sch., Univ. Oregon Health Sci. Cent., Portland, Oreg., USA

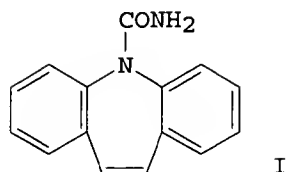
SOURCE: Drug Metab. Dispos. (1978), 6(4), 494-501

CODEN: DMDSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Glucuronide metabolites of carbamazepine (I) [298-46-4] were identified in human urine following chromatog. on XAD-2 resin, permethylation, and combined gas chromatog. and mass spectrometry with an SE-30 capillary column. Eight glucuronide metabolites, previously unidentified in man, were characterized as their permethylated derivs. These included carbamazepine N-glucuronide [60342-79-2], 3 isomers of dihydroxycarbamazepine O-glucuronide, 3 isomers of hydroxymethoxycarbamazepine O-glucuronide and 1 isomer of hydroxycarbamazepine O-glucuronide. Other glucuronide metabolites previously unidentified following enzymatic hydrolysis, were characterized as the unhydrolyzed, permethylated glucuronides, 10,11-dihydro-10,11-dihydroxycarbamazepine O-glucuronide [68011-72-3], and 3 isomers of monohydroxycarbamazepine O-glucuronide.

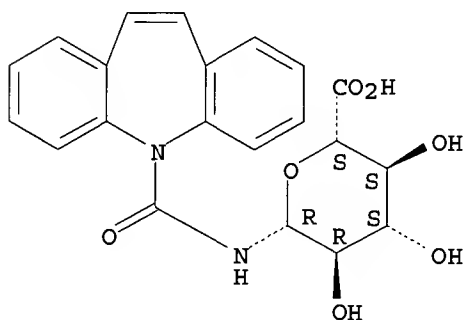
IT 60342-79-2

RL: BIOL (Biological study)  
(as carbamazepine metabolite)

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 76 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:529809 CAPLUS

DOCUMENT NUMBER: 89:129809

TITLE: Ajmaline cardenolide and bufadienolide derivatives

PATENT ASSIGNEE(S): Kharkov Scientific-Research Chemical-Pharmaceutical Institute, USSR

SOURCE: Japan. Kokai, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

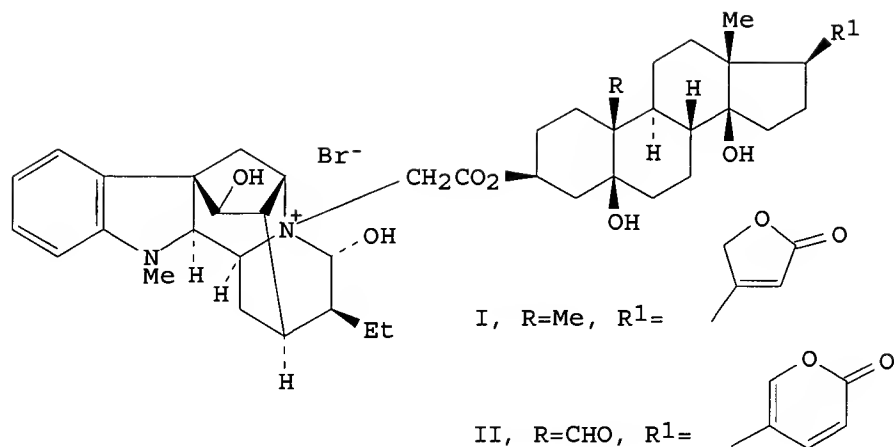
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53052614	A2	19780513	JP 1976-126814	19761023
JP 58009119	B4	19830218		

GI



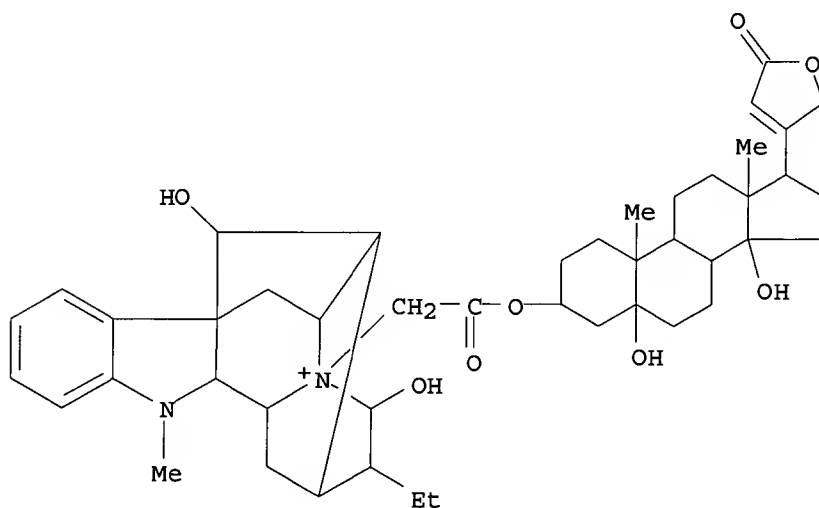
AB Ajmaline reacted with (bromoacetyl)strophanthidin or (bromoacetyl)hellebrigenin to give the corresponding quaternary ammonium compds. (I and II, resp.). Thus, 30 g strophanthidin in dioxane contg. pyridine was treated with BrCH<sub>2</sub>COBr and the resulting 3-O-(bromoacetyl)strophanthidin reacted with equimolar ajmaline in MeCN at room temp. to give 22.4 g I.

IT **67708-31-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 67708-31-0 CAPLUS

CN Ajmalanium, 4-[2-[[[(3.β., 5.β., 14.β.)-21,23-epoxy-5,14-dihydroxy-23-oxo-24-norchol-20(22)-en-3-yl]oxy]-2-oxoethyl]-17,21-dihydroxy-, bromide, (17R,21.α.)- (9CI) (CA INDEX NAME)

PAGE 1-A



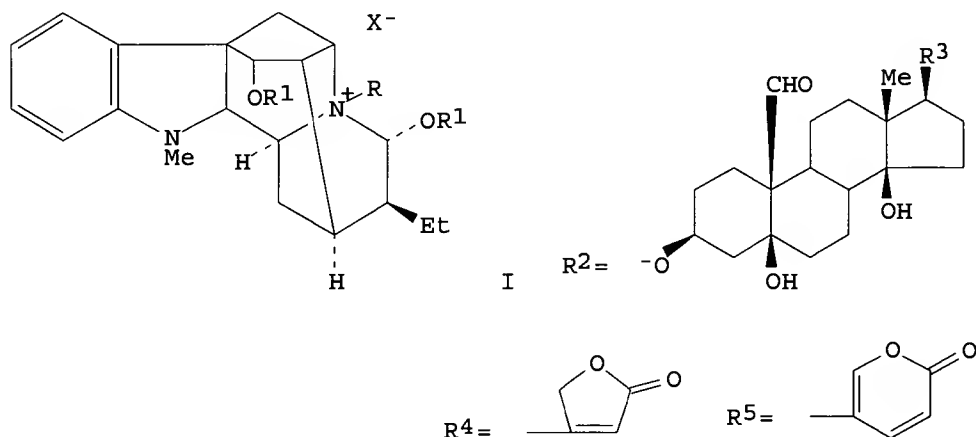
PAGE 2-A

Br<sup>-</sup>

L4 ANSWER 77 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1978:510131 CAPLUS  
 DOCUMENT NUMBER: 89:110131  
 TITLE: Cardenolide and bufadienolide derivatives of ajmaline  
 INVENTOR(S): Makarevich, I. F.; Khadzhai, Ya. I.; Pavlova, V. V.;  
 Nikolaeva, A. V.  
 PATENT ASSIGNEE(S): Kharkov Scientific-Research Chemical-Pharmaceutical  
 Institute, USSR  
 SOURCE: Ger. Offen., 23 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2645873	A1	19780413	DE 1976-2645873	19761011
DE 2645873	B2	19810709		
DE 2645873	C3	19820519		
CH 629506	A	19820430	CH 1976-13105	19761015
PRIORITY APPLN. INFO.:			DE 1976-2645873	19761011

GI



AB The antiarrhythmic (no data) ajmaline derivs. I [R = CH<sub>2</sub>COR<sub>2</sub> (R<sub>3</sub> = R<sub>4</sub>, R<sub>5</sub>); R<sub>1</sub> = H, acyl, C<sub>1</sub>-5 alkyl; X = halide] were prepd. by treatment of cardenolide R<sub>2</sub>H (R<sub>3</sub> = R<sub>4</sub>) or bufadienolide R<sub>2</sub>H (R<sub>3</sub> = R<sub>5</sub>) in an org. solvent with (XCH<sub>2</sub>CO)<sub>2</sub>O (X = halo) at -10.degree. to 5.degree. and the XCH<sub>2</sub>COR<sub>2</sub> was condensed with ajmaline (II). The (XCH<sub>2</sub>CH)<sub>2</sub>O may be replaced with BrCH<sub>2</sub>COBr (III). Thus, 30 g strophanthidin [R<sub>2</sub>H (R<sub>3</sub> = R<sub>4</sub>)] dissolved in pyridine and cooled to 0 to 3.degree. was treated with III to give 26 g BrCH<sub>2</sub>COR<sub>2</sub> (IV). A soln. of 12.5 g II, 19.8g IV, and MeCN stored 40 h at room temp. gave 22 g I [R = CH<sub>2</sub>COR<sub>2</sub> (R<sub>3</sub> = R<sub>4</sub>), R<sub>1</sub> = H, X = Br].

IT 67205-13-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 67205-13-4 CAPLUS

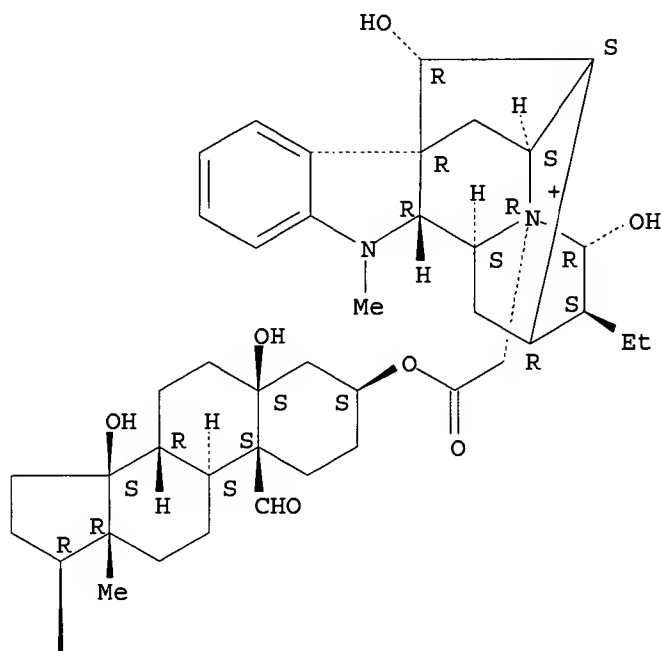
CN Ajmalanum, 4-[2-[[[(3.beta.,5.beta.,14.beta.)-21,23-epoxy-5,14-dihydroxy-19,23-dioxo-24-norchol-20(22)-en-3-yl]oxy]-2-oxoethyl]-17,21-dihydroxy-,

09/ 995,324

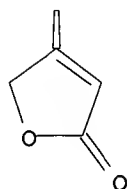
bromide, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A



● Br<sup>-</sup>

L4 ANSWER 78 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:106349 CAPLUS

DOCUMENT NUMBER: 86:106349

TITLE: Synthesis of dibenzo[b,f]cycloprop[d]azepine derivatives. I. Introduction of a cyclopropane ring by the use of Simmons-Smith reagent

AUTHOR(S): Kawashima, Kenya; Kawano, Yasuhiko

CORPORATE SOURCE: Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, Japan

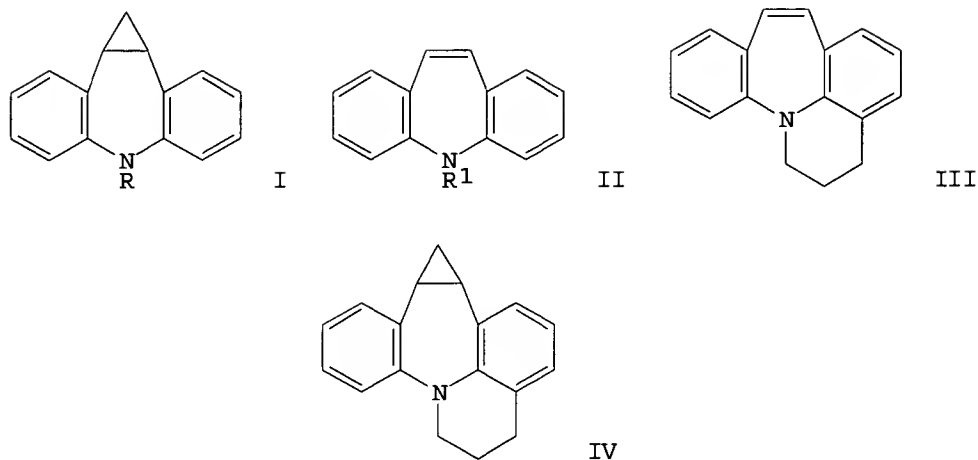
SOURCE: Chem. Pharm. Bull. (1976), 24(11), 2751-60

CODEN: CPBTAL

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

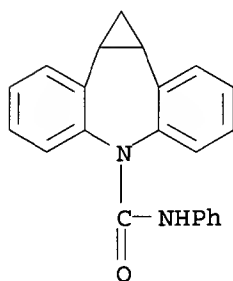


AB The dibenzo[b,f]cycloprop[d]azepine I (R = Me), obtained by Simmons-Smith reaction of the dibenz[b,f]azepine II (R1 = H, Me), was demethylated via I (R = CHO) to give I (R = H), which was converted into the potential anticonvulsant and antidepressant I [R = (CH<sub>2</sub>)<sub>n</sub>NR<sub>2</sub>R<sub>3</sub>, n = 2, 3; R<sub>2</sub>, R<sub>3</sub> = Me, Et, or R<sub>2</sub>R<sub>3</sub> = (CH<sub>2</sub>)<sub>5</sub>, 4-methyl-1-piperazinyl, etc., or R = CONHR<sub>4</sub>, R<sub>4</sub> = H, Me, Ph]. However, cyclopropanation of I [R = (CH<sub>2</sub>)<sub>3</sub>R<sub>5</sub>, R<sub>5</sub> = Br, Cl] with Simmons-Smith reagent gave I (R = allyl, cyclopropylmethyl) and the cyclization products III and IV.

IT **41843-91-8P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and potential anticonvulsants and antidepressants)

RN 41843-91-8 CAPLUS

CN Dibenzo[b,f]cycloprop[d]azepine-6(1H)-carboxamide, 1a,10b-dihydro-N-phenyl-  
 (9CI) (CA INDEX NAME)



L4 ANSWER 79 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:516485 CAPLUS

DOCUMENT NUMBER: 85:116485

TITLE: A new N-glucuronide metabolite of carbamazepine

AUTHOR(S): Bauer, J. E.; Gerber, N.; Lynn, R. K.; Smith, R. G.; Thompson, R. M.

CORPORATE SOURCE: Med. Sch., Univ. Oregon, Portland, Oreg., USA

SOURCE: Experientia (1976), 32(8), 1032-3

CODEN: EXPEAM

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

09/ 995,324

AB Carbamazepine N-glucuronide (I) [60342-79-2] was identified in the bile of isolated perfused rat liver by means of permethylation, gas chromatog., and mass spectrometry.

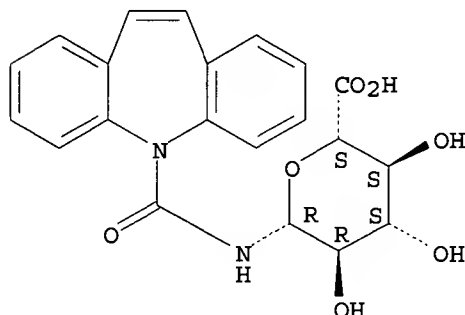
IT 60342-79-2

RL: BIOL (Biological study)  
(as carbamazepine metabolite)

RN 60342-79-2 CAPLUS

CN .beta.-D-Glucopyranuronic acid, 1-deoxy-1-[(5H-dibenz[b,f]azepin-5-ylcarbonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 80 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:446267 CAPLUS

DOCUMENT NUMBER: 85:46267

TITLE: 10,11-Dihydro-10,11-etheno-5H-dibenz[b,f]-azepines and 10,11-dihydro-10,11-etheno-5H-dibenzo[a,d]-cycloheptenes, and derivatives thereof

PATENT ASSIGNEE(S): Syntex Corp., Panama

SOURCE: Brit., 38 pp.  
CODEN: BRXXAA

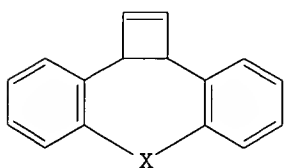
DOCUMENT TYPE: Patent

LANGUAGE: English

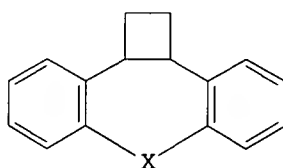
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1428481	A	19760317	GB 1973-30267	19730626
PRIORITY APPLN. INFO.: GI			US 1972-270663	19720711



I



II

AB The title compds. I [X = N(CH<sub>2</sub>)<sub>3</sub>NHMe, C:CH(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>, CHC.tplbond.CCH<sub>2</sub>NHMe, C:C:CHCH<sub>2</sub>NHMe, CHC.tplbond.CCH<sub>2</sub>NMeCH<sub>2</sub>COC<sub>6</sub>H<sub>4</sub>Cl-4, C:NO(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>, 3-(N'-.beta.-hydroxyethylpiperazino)prop-1-ynylmethylene] and II [X = N(CH<sub>2</sub>)<sub>3</sub>NHMe, C:CH(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>], useful as antidepressants (no data), were prepd. from 5-formyl-5H-dibenz[b,f]azepine or 5H-dibenzo[a,d]cyclohepten-5-one, initially by irradiation with maleic anhydride and decarboxylation.



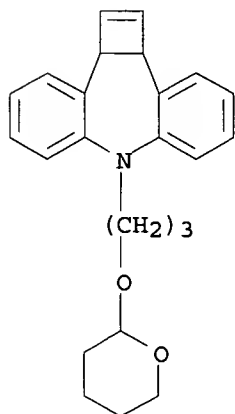
09/ 995,324

IT 60549-21-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate in (methylaminopropyl)dihydroethenodibenzazepine prepn.)

RN 60549-21-5 CAPLUS

CN 7H-Dibenzo[b,f]cyclobut[d]azepine, 2a,11b-dihydro-7-[3-[(tetrahydro-2H-pyran-2-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



3'-diethylamino-2'-hydroxypropyl, 3'-piperidino-2'-hydroxypropyl, 3'-morpholino-2'-hydroxypropyl, and 3'-pyrrolidino-2'-hydroxypropyl substituents were the most active. The LD50:ED20 (20% effective dose) ratios for the 14 most active compds. ranged from 7.9 to 23.2.

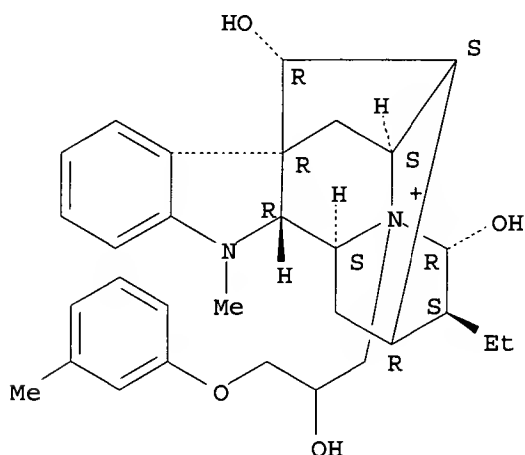
IT 58892-94-7

RL: BIOL (Biological study)  
(heart arrhythmia response to)

RN 58892-94-7 CAPLUS

CN Ajmalanum, 17,21-dihydroxy-4-[2-hydroxy-3-(3-methylphenoxy)propyl]-, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 82 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1973:521733 CAPLUS

DOCUMENT NUMBER: 79:121733

TITLE: Formation of N-glucuronide of demethylimipramine in the dog

AUTHOR(S): Bickel, M. H.; Minder, R.; Di Francesco, C.

CORPORATE SOURCE: Med. Chem. Inst., Univ. Bern, Bern, Switz.

SOURCE: Experientia (1973), 29(8), 960-1

CODEN: EXPEAM

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thin-layer chromatog. of urine and bile from dogs given demethylimipramine (I) [50-47-5] (10.0 mg/kg, oral) or imipramine [50-49-7] (4.55 mg/kg, oral) revealed a previously unreported I conjugate. The response of this conjugate to various conditions of hydrolysis indicates it is demethylimipramine N-glucuronide [42583-83-5].

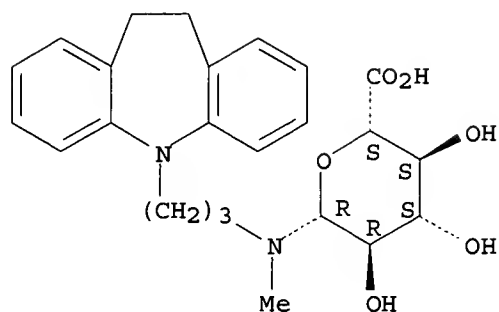
IT 42583-83-5

RL: BIOL (Biological study)  
(demethylimipramine metabolite)

RN 42583-83-5 CAPLUS

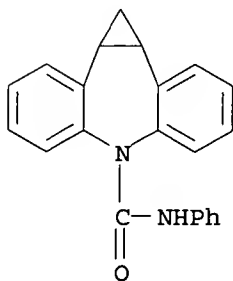
CN 5H-Dibenz[b,f]azepine-5-propanamine, N-.beta.-D-glucopyranuronosyl-10,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1973:431953 CAPLUS  
 DOCUMENT NUMBER: 79:31953  
 TITLE: 1,1a,6,10b-Tetrahydrocyclopropa[a]dibenz[b,f]azepin-6-carboxamides  
 INVENTOR(S): Morita, Katsura; Kawashima, Takeya  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.  
 SOURCE: Jpn. Tokkyo Koho, 3 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 48008631	B4	19730316	JP 1970-105337	19701127
GI	For diagram(s), see printed CA Issue.				
AB	The title compds. I were prepd. by treating 1,1a,6,10b-tetrahydrocyclopropa[d]dibenz[b,f]azepine (II) with isocyanic acid or its esters. I were anticonvulsants, antiepileptics, and remedies for trigeminal neuralgia. E.g., refluxing II and MeNCO in xylene 24 hr gave 58% I (R = Me). I (R = Ph) and I (R = H) were also prepd.				
IT	<b>41843-91-8P</b>				
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	41843-91-8 CAPLUS				
CN	Dibenzo[b,f]cycloprop[d]azepine-6(1H)-carboxamide, 1a,10b-dihydro-N-phenyl-(9CI) (CA INDEX NAME)				



L4 ANSWER 84 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1973:405322 CAPLUS  
 DOCUMENT NUMBER: 79:5322  
 TITLE: 1a, 10b-Dihydro-6H-dibenz[b,f]oxireno[d]azepine-6-

carboxamides  
 INVENTOR(S): Kawashima, Kenya; Ishiguro, Toshihiro  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.  
 SOURCE: Ger. Offen., 15 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2246842	A1	19730405	DE 1972-2246842	19720923
JP 54039390	B4	19791127	JP 1971-76971	19710930
JP 48039488	A2	19730609		
JP 49031685	A2	19740322	JP 1972-74448	19720724
JP 55017036	B4	19800508		
JP 49031686	A2	19740322	JP 1972-76324	19720728
AU 7247034	A1	19740411	AU 1972-47034	19720925
US 3842091	A	19741015	US 1972-291627	19720925
AT 323184	B	19750625	AT 1972-323184	19720925
AT 323179	B	19750625	AT 1972-8219	19720925
BE 789320	A1	19730327	BE 1972-122442	19720927
NL 7213177	A	19730403	NL 1972-13177	19720928
FR 2154714	A1	19730511	FR 1972-34446	19720928
GB 1402325	A	19750806	GB 1972-44772	19720928
NO 136495	B	19770606	NO 1972-3480	19720928
HU 164851	P	19740411	HU 1972-TA1212	19720929
ES 407133	A1	19751016	ES 1972-407133	19720929
CA 981667	A1	19760113	CA 1972-152881	19720929
CH 575950	A	19760531	CH 1972-14280	19720929
CH 578569	A	19760813	CH 1975-16155	19720929
PRIORITY APPLN. INFO.:			JP 1971-76971	19710930
			JP 1972-74448	19720724
			JP 1972-76324	19720728

GI For diagram(s), see printed CA Issue.

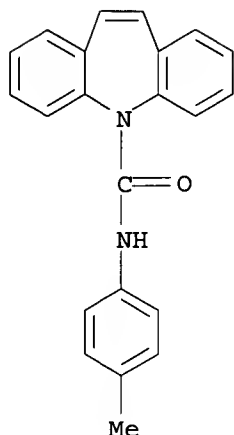
AB Seven title compds. [I; R = H, NH<sub>2</sub>, Me, Pr, (CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, CH<sub>2</sub>Ph, or C<sub>6</sub>H<sub>4</sub>Me-p], useful as anticonvulsive, antiepileptic, antiarrhythmic, and antineuralgic agents, were prepd. by reaction of II with RNH<sub>2</sub> and reaction of resulting III with percarboxylic acids (AcOOH or m-ClC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>OH), or by reaction of II with percarboxylic acids and reaction of the resulting IV (XY = O) with RNH<sub>2</sub> or successively with HCl or HBr and RNH<sub>2</sub> via IV (X = Cl, Br, Y = OH).

IT **41359-03-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 41359-03-9 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, N-(4-methylphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1973:4398 CAPLUS

DOCUMENT NUMBER: 78:4398

TITLE: Amino alcohol derivatives of ajmaline

INVENTOR(S): Braun, Klaus; Gabsch, Guenther; Femmer, Klaus; Ertel, Rolf; Foerster, Werner

SOURCE: Ger. (East), 3 pp. Addn. to Ger. (East) 82,731 (CA 77;19864w).

CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 91507		19720720	DD 1970-152344	19701231

GI For diagram(s), see printed CA Issue.

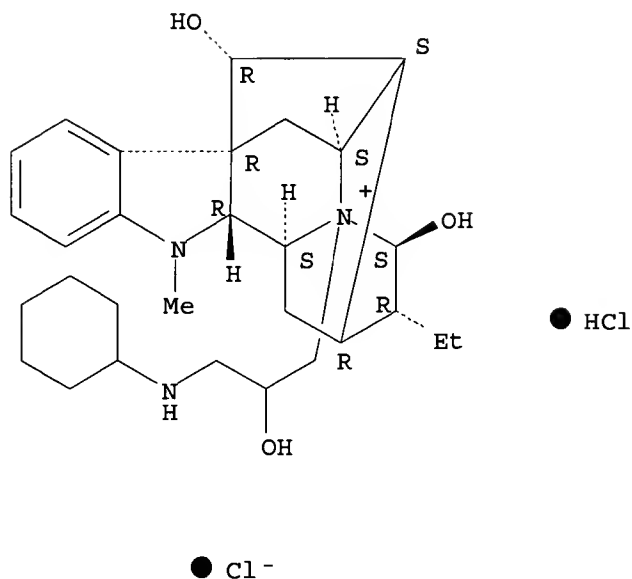
AB Ajmaline or isoajmaline was treated with 2,3-epoxypropylamines to give a 1:1 mixt. of the quaternary ajmalinium and isoajmalinium salts (I, R = R<sub>1</sub> = Et, Me<sub>2</sub>CHCH<sub>2</sub>; R = H, R<sub>1</sub> = Me<sub>2</sub>CH, cyclohexyl; RR<sub>1</sub># = piperidino, morpholino, pyrrolidino; X = Cl tartrate).

IT **41258-69-9P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 41258-69-9 CAPLUS

CN Ajmalanum, 4-[3-(cyclohexylamino)-2-hydroxypropyl]-17,21-dihydroxy-, chloride, monohydrochloride, (17R,20.alpha.,21.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 86 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:500563 CAPLUS

DOCUMENT NUMBER: 77:100563

TITLE: Transannular cyclization of cycloolefinic N-chloro amines. Synthesis of azabicyclic compounds

AUTHOR(S): Bastable, J. W.; Hobson, J. D.; Riddell, W. D.

CORPORATE SOURCE: Chem. Dep., Univ. Birm., Birmingham, Engl.

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1972), (17), 2205-13  
CODEN: JCPRB4

DOCUMENT TYPE: Journal

LANGUAGE: English

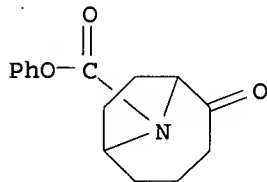
AB N-Chloro-N-methyl-4-cyclooctenamine and N-chloro-N-methyl-4-cycloheptenamine cyclized in the presence of various catalysts (e.g. AgClO<sub>4</sub>) and solvents (e.g. Me<sub>2</sub>CO) to give 2-substituted N-bridged bicyclic compds. Cis addn. predominated in the cyclooctenamine. A radical chain mechanism was suggested.

IT **38288-98-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 38288-98-1 CAPLUS

CN 9-Azabicyclo[4.2.1]nonane-9-carboxylic acid, 2-oxo-, phenyl ester (9CI)  
(CA INDEX NAME)



L4 ANSWER 87 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:419864 CAPLUS

DOCUMENT NUMBER: 77:19864

TITLE: Amino alcohol derivatives of ajmaline

09/ 995,324

INVENTOR(S): Braun, Klaus; Gabsch, Guenther; Foerster, Werner;  
Ertel, Rolf; Femmer, Klaus  
SOURCE: Ger. (East), 4 pp.  
CODEN: GEXXA8  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DD 82731		19710620	DD 1969-141478	19690728

GI For diagram(s), see printed CA Issue.

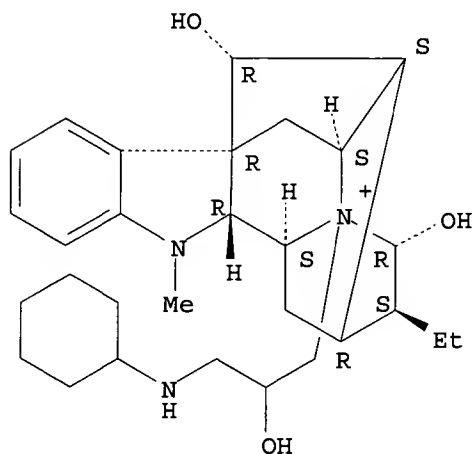
AB Nine antiarrhythmic title compds. I, R = Et<sub>2</sub>N, 1-pyrrolidinyl, piperidino, morpholino, Me<sub>2</sub>CHNH, cyclohexylamino, (Me<sub>2</sub>CHCH<sub>2</sub>)<sub>2</sub>N; X = Cl, tartrate| were prepd. by reacting the corresponding epoxypropane (II) with ajmaline. Thus, ajmaline in EtOH was heated 6 hr at 75.degree. with II (R = Et<sub>2</sub>N), the product taken up in dioxane, and treated with ether-HCl to ppt. I (R = Et<sub>2</sub>N, X = Cl). I (R = 1-pyrrolidinyl, X = tartrate) showed an ED<sub>20</sub>/LD<sub>50</sub> of 23.2 (by aconitine test on rats), much higher than that of N-propylajmaline, but it showed little neg. inotropic effect at 0.1 and 0.4 mg/kg (on dogs), which compared favorably with the latter.

IT **32537-78-3P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 32537-78-3 CAPLUS

CN Ajmalanum, 4-[3-(cyclohexylamino)-2-hydroxypropyl]-17,21-dihydroxy-, chloride, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1972:85990 CAPLUS  
DOCUMENT NUMBER: 76:85990  
TITLE: Ajmaline derivatives  
INVENTOR(S): Braun, Klaus; Gabsch, Guenther; Foerster, Werner;  
Femmer, Klaus  
SOURCE: Ger. (East), 4 pp.  
CODEN: GEXXA8

09/ 995,324

DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DD 77981		19701205	DD	19690728

GI For diagram(s), see printed CA Issue.

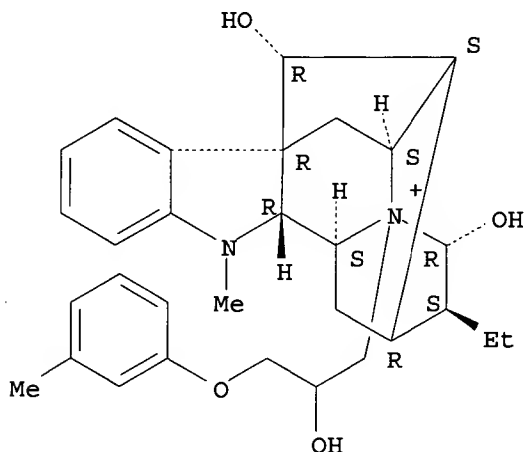
AB The ajmaline derivs. I (R = Me, Et, Pr, CHMe2, Bu, m-MeC6H4, .alpha.-naphthyl) are prepd. by treating ajmaline with a suitably substituted epoxypropane or epichlorohydrin. The antiarrhythmic ED20 of I (R = Et, m-MeC6H4) are 0.26 and 0.66 mg/kg, resp., compared with 2.13 mg/kg for ajmaline and 0.17 mg/kg for N-propylajmaline. The LD50 of the 4 compds. are 2.9, 11.2, 26.0, and 1.4 mg/kg, resp. I (R = Et) is obtained in 82% yield by refluxing ajmaline with 1-ethoxy-2,3-epoxypropane.

IT **35527-52-7P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 35527-52-7 CAPLUS

CN Ajmalanum, 17,21-dihydroxy-4-[2-hydroxy-3-(3-methylphenoxy)propyl]-, chloride, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



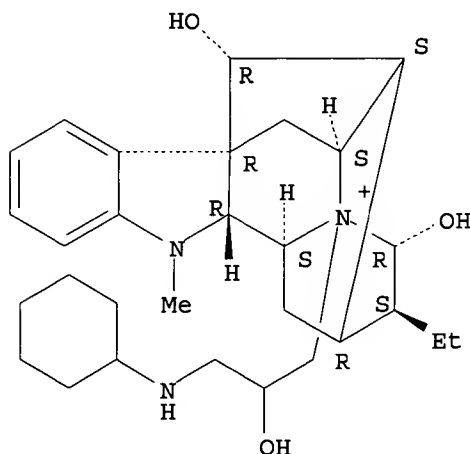
● Cl<sup>-</sup>

L4 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1971:529991 CAPLUS  
DOCUMENT NUMBER: 75:129991  
TITLE: Ajmaline derivatives  
INVENTOR(S): Braun, Klaus; Gabsch, Guenther; Foerster, Werner;  
Ertel, Rolf; Femmer, Klaus  
PATENT ASSIGNEE(S): VEB Arzneimittelwerk Dresden  
SOURCE: Brit., 4 pp.  
CODEN: BRXXAA  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:



	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	GB 1244597		19710902	GB	19700507
GI	For diagram(s), see printed CA Issue.				
AB	The antiarrhythmic title compds. (I) were prepd. and tested on dogs. Thus, ajmaline was refluxed 6 hr in EtOH with 1-(diethylamino)-2,3-epoxypropane and treated with Et <sub>2</sub> O-HCl after chromatog. to give 70% I (R = NEt <sub>2</sub> , X = Cl) hydrochloride. Similarly prepd. were I (X- = tartrate; R = morpholino, pyrrolidino, piperidino) and I (X = Cl, R = piperidino, morpholino, Me <sub>2</sub> CHNH, isoBu <sub>2</sub> N, cyclohexylamino).				
IT	32537-78-3P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	32537-78-3 CAPLUS				
CN	Ajmalanum, 4-[3-(cyclohexylamino)-2-hydroxypropyl]-17,21-dihydroxy-, chloride, (17R,21.alpha.)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 90 OF 96 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1971:436442 CAPLUS  
 DOCUMENT NUMBER: 75:36442  
 TITLE: Antiarrhythmic 4-[3-(diethylamino)-2-hydroxypropyl]ajmalinium salts  
 INVENTOR(S): Braun, Klaus; Gabsch, Guenther; Foerster, Werner; Ertel, Rolf; Femmer, Klaus  
 PATENT ASSIGNEE(S): VEB Arzneimittelwerk Dresden  
 SOURCE: Ger. Offen., 6 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2025286	A	19710218	DE 1970-2025286	19700523
DE 2025286	B2	19760304		
DE 2025286	C3	19761021		

09/ 995,324

AT 293629	B	19711025	AT 1970-4728	19700526
SU 399125	D	19730927	SU 1970-1452692	19700625
FR 2059563	A1	19710604	FR 1970-24993	19700706

PRIORITY APPLN. INFO.:

DD 1969-141478 19690728

GI For diagram(s), see printed CA Issue.

AB The compatible title salts (I) were prepd. Thus, heating ajmaline and 1-(diethylamino)-2,3-epoxypropane 6 hr at 75.degree. and treatment with HCl gave 70% I.HCl (R = Et<sub>2</sub>N, X = Cl). Similarly prepd. were I (R and X given): 1-pyrrolidinyl, tartrate; piperidino, Cl; piperidino, tartrate; morpholino, Cl; (iso-Bu)<sub>2</sub>N, Cl.

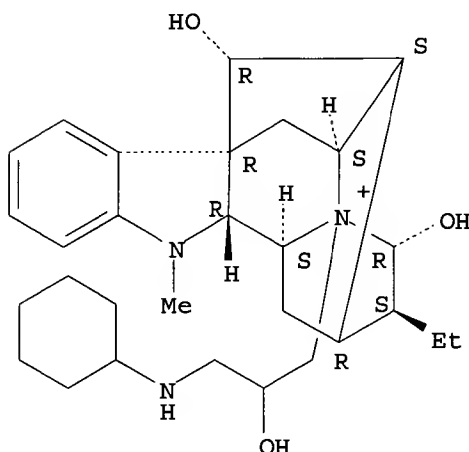
IT 32537-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 32537-78-3 CAPLUS

CN Ajmalanum, 4-[3-(cyclohexylamino)-2-hydroxypropyl]-17,21-dihydroxy-, chloride, (17R,21.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

L4 ANSWER 91 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:43726 CAPLUS

DOCUMENT NUMBER: 72:43726

TITLE: Selected 13,14-diazatricyclo-[6.4.1.12,7]tetradecanes and diazatricyclo[6.4.1.12,7] tetradecatetraenes

INVENTOR(S): Johnson, Alexander L.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.

SOURCE: U.S., 11 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3475433	A	19691028	US 1966-529961	19660225

GI For diagram(s), see printed CA Issue.

AB The title compds., useful as adhesives, are prepd. by thermal rearrangement of 1H-azepine-1-carbonitrile dimers to give the tetraenes,

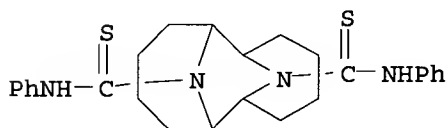
which are hydrogenated to give the tetradecanes. Thus, 200 g powd. I was added in 10 min at 140.degree. to 1000 g naphthalene flushed with N, and was heated at 210.degree. for 20 min. The mixt. was cooled to 100.degree., dild. with 2500 ml C6H6, cooled to 60.degree., and filtered. The residue was washed with 1250 ml C6H6 and dried to give 69% cryst. II (R = CN) (III). III, m. >39.degree. (decompn.) was also prepd. by heating I, with or without NaCl, in an auger reactor at 250.degree. for 3 hr. III (5.6 g) was heated with 50 ml 50% H2SO4 at 100.degree. for 6 hr, and the insol. product was washed with H2O and 4.48 g was recrystd. twice from 20 ml aq. dichlorotetrafluoroacetone hydrate to give 53% II (R = CONH2) (IV), m. >29.degree. (decompn.). III and H2SO4 were heated, the mixt. was freed of IV, and the aq. filtrate was treated with NaHCO3 and extd. with CHCl3. The exts. were evapd. to give II (R = H) (V), m. 145-6.5.degree. (decompn.). V was shaken with NaOH and BzCl to give II (R = Bz), m. 310-11.degree. (decompn.). II (R = PhNHCO), m. >35.degree. (decompn.), II (R = p-BrC6H4CO), m. 322-3.degree. (decompn.), II (R = Ph-NHCS), m. 211-12.degree. (decompn.), II (R = Me), m. 166.5-8.0.degree. (decompn.), and II.2HCl (R = H) (VI), m. >30.degree. (decompn.) were similarly prepd. V (300 mg) in a mixt. of H2O 10, MeOH 10, and concd. HCl 0.5 ml was hydrogenated at 25.degree./760 mm over Pt oxide to give 239 mg VII.2HCl (R = H), m. >32.degree., which was treated with NaOH to give VII (R = H) (VIII), m. 61-2.degree.. VII.2HBr (R = H), m. >32.degree. (decompn.), VII (R = Bz), m. 319.5-20.5.degree., VII (R = PhNHCS), m. 289-9.5.degree. (decompn.), VII (R = PhNHCO), m. 374-5.degree. (decompn.), and VII (R = Me), m. 95-6.degree. were prepd. similarly. VI was treated with NaNO2 and concd. HCl to give II (R = NO), m. >25.degree. (decompn.). VII (R = NO), m. 180-2.5.degree. (decompn.) and II (R = EtOCO), m. 19 6.5-7.5.degree., were similarly prepd. from VIII and V, resp. A suspension of 0.27 g V in 10 ml CH2Cl2, 40 ml H2O, and 0.12 g NaOH was treated with 0.25 g adipoyl chloride, stirred 10 min, freed of CH2Cl2, cooled to 0.degree., and filtered. V-adipic acid copolymer (IX), m. >33.degree., was obtained as the residue. VIII-adipic acid copolymer (X), m. >31.degree. (decompn.) was also prepd. X and IX gave self-supporting but brittle films. Suberoyl chloride, sebacoyl chloride, and ethylene glycol bis(chloroformate) were also used as monomers. The compds. melted with decompn. to give gummy products useful as adhesives.

IT 24402-55-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 24402-55-9 CAPLUS

CN 13,14-Diazatricyclo[6.4.1.12,7]tetradecane-13,14-dicarboxanilide, dithio-(8CI) (CA INDEX NAME)



L4 ANSWER 92 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:467252 CAPLUS

DOCUMENT NUMBER: 69:67252

TITLE: Dibenzazepines with basic substituents

PATENT ASSIGNEE(S): Geigy, J.R., A.-G.

SOURCE: Fr., 13 pp.

CODEN: FRXXAK

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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FR 1463803		19661230		
PRIORITY APPLN. INFO.:		CH		19631216

GI For diagram(s), see printed CA Issue.

AB Various means of prepg. dibenzazepines with the general formula I are described. Thus, 141 g. I (R = Ac, R1 = R2 = O) in 200 ml. 38% CH<sub>2</sub>O was hydrogenated over Raney Ni at 40-50.degree. and 30 atm. 9 hrs. to give I (R = Ac, R1 = R2 = Me), m. 130-2.degree.. This compd. (280.3 g.) was stirred 8 hrs. at 170.degree. with 73 g. KOH in 300 ml. diethylene glycol monoethyl ether (II), cooled to 130-40.degree., and dild. with 1.5 l. ice water to give I (R = H, R1 = R2 = Me) (III), m. 103-5.degree.. A suspension of 50.5 g. I (R = Ac, R2 = R1 = H) (IV) and 55.3 g. K<sub>2</sub>CO<sub>3</sub> in 250 ml. Me<sub>2</sub>CO was treated with 170 g. MeI, refluxed 12 hrs., and filtered to give I.MeI (R = Ac, R1 = R2 = Me), m. 185-7.degree.. This compd. (21.1 g.) was refluxed with 7.3 g. KOH in 75 ml. II as above to give III. IV (252 g.) was heated 8 hrs. at 170.degree. with 73 g. KOH in 200 ml. II to give I (R = R1 = R2 = H), m. 98-100.degree.. This compd. (420 g.) was refluxed 48 hrs. in 1 l. HCO<sub>2</sub>Et with 0.5 ml. HOAc and 1 ml. pyridine, stripped of 600 ml. HCO<sub>2</sub>Et, and dild. with 400 ml. Et<sub>2</sub>O to give I (R = R1 = H, R2 = CHO), m. 121-3.degree.. This compd. (120 g.) in 300 ml. tetrahydrofuran was refluxed 12 hrs. with 38.5 g. LiAlH<sub>4</sub> in 700 ml. ether, made alk., extd. with CH<sub>2</sub>Cl<sub>2</sub>, and chromatographed on Al<sub>2</sub>O<sub>3</sub> to give I (R = R1 = H, R2 = Me), m. 87-9.degree.. A soln. of 143 g. III in 800 ml. PhMe was treated with 88 ml. 33% NaNH<sub>2</sub> in PhMe at 80.degree., heated to boiling, refluxed 2 hrs., cooled to 70.degree., mixed with 123 g. 3-dimethylaminopropyl chloride hydrochloride in 600 ml. PhMe added in 90 min., refluxed 12 hrs., and dild. with 50 ml. water. The mixt. was extd. with PhMe and the ext. concd., taken up in 200 ml. Et<sub>2</sub>O, and extd. with 250 ml. 2N HOAc and 100 ml. 0.5N NaH<sub>2</sub>PO<sub>4</sub>. The acid exts. were made alk., extd. with 2:1 ether-CH<sub>2</sub>Cl<sub>2</sub>, stripped of solvent, and chromatographed on Al<sub>2</sub>O<sub>3</sub> to give I.2HCl [R = (CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, R1 = R2 = Me], m. 195-200.degree.. Other I (R1 = R2 = Me) were prepd. similarly (R, salt, and m.p. given): (CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>, HCl, 214-16.degree.; CH<sub>2</sub>CHMeCH<sub>2</sub>NMe<sub>2</sub>, 2HCl, 203-5.degree.; CH<sub>2</sub>CH(NMe<sub>2</sub>)Me, HCl, 210-12.degree.; 2-(1-methyl-2-piperidyl)ethyl, -, 64-6.degree.; 3-piperidinopropyl, -, -; 3-(4-methyl-1-piperazinyl)propyl, 3HCl, 215-20.degree.. A soln. of 41.2 g. CH<sub>2</sub>BrCHMeCH<sub>2</sub>Cl in 150 ml. PhMe was treated with 8.8 g. NaNH<sub>2</sub> in 150 ml. PhMe added dropwise in 10 min. and 47.7 g. III in 200 ml. PhMe added dropwise in 90 min. at 90.degree. and refluxed 12 hrs. to give crude I (R = CH<sub>2</sub>CHMeCH<sub>2</sub>Cl, R1 = R2 = Me). This product was taken up in 100 ml. HCONMe<sub>2</sub> and heated 16 hrs. at 120.degree. with 25.5 g. 1-hydroxyethylpiperazine and 25.5 g. K<sub>2</sub>CO<sub>3</sub> to give 1-3-(3-dimethylamino-10,11-dihydro-5H - dibenz [b,f] azepin - 10 - yl) - 2 - methylpropylpiperazine-4-ethanol trihydrochloride, m. 221-3.degree.. Similarly prepd. was 5-[3-(1-hydroxyethyl-4-piperazinyl)propyl]-3-dimethylamino-10,11-dihydro-5H-dibenz [b,f]azepine dimaleate, m. 138-40.degree.. A soln. of 26.8 g. I [R = (CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, R1 = R2 = Me] in 150 ml. C<sub>6</sub>H<sub>6</sub> was refluxed 20 hrs. with 9.85 g. ClCO<sub>2</sub>Et in 30 ml. C<sub>6</sub>H<sub>6</sub> to give Et N-[3-(3-dimethylamino-10,11-dihydro - 5H - dibenz [b,f]azepin - 5 - yl)propyl] - N - methylcarbamate. This crude ester was treated with KOH and II as above to give I.2HCl [R = (CH<sub>2</sub>)<sub>3</sub>NHMe, R1 = R2 = Me], m. 197-200.degree.. Similarly prepd. was I (R = CH<sub>2</sub>CHMeCH<sub>2</sub>NHMe, R1 = R2 = Me); oxalate m. 162-5.degree.. I (R = R1 = H, R2 = Me) (11.2 g.) was treated with NaNH<sub>2</sub> and Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl hydrochloride as above to give I (R = CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R1 = H, R2 = Me), b0.007 151-60.degree.. Similarly prepd. was I [R = (CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, R1 = H, R2 = Me], m. 77-80.degree.. I (R = H, R1 = Ac, R2 = Me) was condensed with Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl hydrochloride and NaNH<sub>2</sub> as above to give an oily product which was treated with ClCO<sub>2</sub>Et and II to give I.HCl (R = CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R1 = H, R2 = Me), m. 223-5.degree.. III (23.8 g.) was condensed with N-benzyl-N-phenylisopropylaminoethyl chloride hydrochloride and NaNH<sub>2</sub> as above to give a crude base which was hydrogenated over Pd-C to give I.2HCl

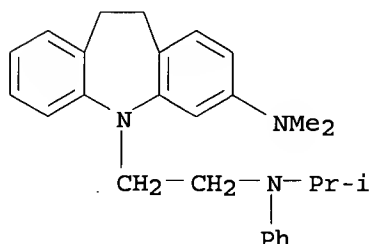
(R = CH<sub>2</sub>CH<sub>2</sub>NPhPr-iso, R<sub>1</sub> = R<sub>2</sub> = Me), m. 211-13.degree.. Condensation of 3-dimethylamino-5H-dibenz[b,f]azepine with Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>Cl and NaNH<sub>2</sub> as above gave 5-(3-dimethylaminopropyl)-3-dimethylamino-5H-dibenz[b,f]azepine, m. 174-6.degree.. This compd. was treated with ClCO<sub>2</sub>Et in C<sub>6</sub>H<sub>6</sub> to give a carbamic ester which was dissolved in Carbitol, heated 16 hrs. with 20 g. KOH at 170.degree., and chromatographed to give 5-(3-methylaminopropyl)-3-dimethylamino-5H-dibenz[b,f]azepine; oxalate m. 164-6.degree.. I [R = (CH<sub>2</sub>)<sub>3</sub>NMeCO<sub>2</sub>Et, R<sub>1</sub> = R<sub>2</sub> = Me] was reduced with LiAlH<sub>4</sub> as above to give I.2HCl [R = (CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, R<sub>1</sub> = R<sub>2</sub> = Me], m. 198-200.degree.. The same product was obtained by treatment of I [R = (CH<sub>2</sub>)<sub>3</sub>NHMe, R<sub>1</sub> = R<sub>2</sub> = Me] with HCO<sub>2</sub>Et and redn. of the product with LiAlH<sub>4</sub>. III (23.8 g.) in 150 ml. PhMe was treated with 0.12 mole NaH at 90.degree. and the base obtained from 34.4 g. benzylmethylaminopropyl chloride oxalate to give an oily product, which was hydrogenated over Pd/C to give I [R = (CH<sub>2</sub>)<sub>3</sub>NHMe, R<sub>1</sub> = R<sub>2</sub> = Me], m. 198-200.degree..

IT 19373-56-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 19373-56-9 CAPLUS

CN 5H-Dibenz[b,f]azepine, 3-(dimethylamino)-10,11-dihydro-5-[2-(N-isopropylanilino)ethyl]-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

L4 ANSWER 93 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:419000 CAPLUS

DOCUMENT NUMBER: 69:19000

TITLE: The synthesis and pharmacological study of acyl derivatives of iminodibenzyl

AUTHOR(S): Bagal, V. N.; Kvitko, I. Ya.; Lapin, I. P.; Porai-Koshits, B. A.; Favorskii, O. V.

CORPORATE SOURCE: Leningr. Tekhnol. Inst. im. Lensovet, Leningrad, USSR  
SOURCE: Khim.-Farm. Zh. (1967), 1(12), 21-6

CODEN: KHFZAN

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The treatment of 10,11-dihydro-5H-dibenz[b,f]azepine (I) with halopropionyl chlorides and subsequently with primary or secondary amines, afforded II and IIa, resp. Treating 2 g. I and 1.3 g. freshly distd. ClCH<sub>2</sub>CH<sub>2</sub>COC<sub>2</sub>H<sub>5</sub> in anhyd. C<sub>6</sub>H<sub>6</sub> gave 2.37 g. N-(.beta.-chloropropionyl)-10,11-dihydro-5H-dibenz[b,f]azepine (III), m. 105-6.degree. (EtOH). Similarly, 7.5 g. I and 7.4 g. BrCH<sub>2</sub>CHMeCOC<sub>2</sub>H<sub>5</sub> gave 11.8 g. N-(.beta.-bromo-.alpha.-methylpropionyl)-10,11-dihydro-5H-dibenz[b,f]azepine, m. 118.5.degree. (cyclohexane). A soln. of 2.85 g. III in 70 ml. anhyd. PhMe was treated with 2.02 g. iso-Pr<sub>2</sub>NH, the mixt. refluxed 18 hrs., the solid removed, and the filtrate evapd. to give an oily residue which was dissolved in anhyd. Et<sub>2</sub>O and treated with HCl-satd. Et<sub>2</sub>O to give 1.7 g. II

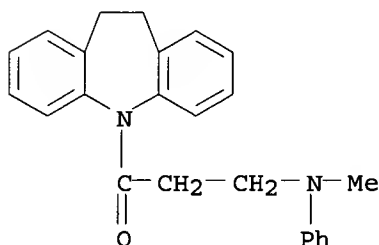
(R = H, R' = R" = iso-Pr, X = HCl) (IIb), m. 187-8.degree. (iso-PrOH). Analogously were prepd. the following II (R, R', R", X, m.p., and % yield given): H, H, Me, HCl, 167.degree. (decompn.) (EtOH), 20; H, Me, Me, HCl, 165-7.degree. (EtOH-Et2O), 87; H, Et, HCl, 168-70.degree. (EtOH-Et2O), 40; H, Bu, Bu, (CO2H)2, 126-7.degree. (EtOH-Et2O), 54.5; H, Me, Ph, HCl, 172-4.degree. (iso-PrOH), 33; (CH2)2OH, PhCH2, (CO2H)2, 170-2.degree. (EtOH), 75; Me, Me, Me, HCl, 240-1.degree. (MeOH), 43; Me, Et, Et, HCl, 230-1.degree. (MeOH), 52; H, H, (CH2)2OCH2Ph, -, 101-3.degree., -. Also prepd. were the following IIa (R, R', X, m.p., and % yield given): H, 4-morpholinyl, HCl, 205-6.degree. (EtOH), 54.6; H, 1-methyl-4-piperazinyl, HCl, 227-32.degree. (EtOH), 83; H, 1-(.beta.-hydroxyethyl)-4-piperazinyl, 2HCl (IIc), 130.degree. (iso-PrOH), 51; H, 1-piperidinyl, HCl, 158-9.degree. (iso-PrOH), 67.5; Me, 1-piperidinyl, HCl, 248.degree. (iso-PrOH), 50; Me, 4-morpholinyl, HCl, 250-1.degree. (iso-PrOH), 39. A 1:1 mixt. of III and N-(.beta.-hydroxyethyl)piperazine gave IV, m. 238-8.5.degree. (MeOH), as opposed to a 1:6 mixt. which gave only IIc. A soln. of 0.85 g. III in 15 ml. anhyd. C6H6 was treated with 0.75 g. MeNH2 in 5 ml. C6H6, the mixt. kept 7 days, refluxed 2 hrs., the solid removed, the filtrate worked up as for IIb to give an oily product which was dissolved in an alc. and pptd. with petroleum ether to give 0.5 g. V, m. 137.degree. (decompn.). The reaction of 2.85 g. III and 2.67 g. N-methylpyridone gave 1.25 g. N-acryloyl-10,11-dihydro-5H-dibenz[b,f]azepine, m. 97-8.degree. (iso-PrOH). The compds. exhibited adrenopos., cholinoneg., and antireserpine action in rats and mice.

IT 19055-31-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 19055-31-3 CAPLUS

CN 5H-Dibenz[b,f]azepine, 10,11-dihydro-5-(N-methyl-N-phenyl-.beta.-alanyl)-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

L4 ANSWER 94 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:105032 CAPLUS

DOCUMENT NUMBER: 68:105032

TITLE: Heterocyclic derivatives

INVENTOR(S): Renz, Jany; Bourquin, Jean P.; Winkler, Hans;  
Brueschweiler, Conrad; Ruesch, Leo; Schwarb, Gustav

PATENT ASSIGNEE(S): Sandoz Ltd.

SOURCE: Patentschrift (Switz.), 2 pp.

CODEN: SWXXAS

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO. DATE

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	CH 433329	19670930	CH	19631024
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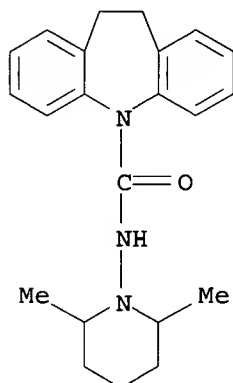
GI For diagram(s), see printed CA Issue.

AB The treatment of a heterocyclic amino compd. such as 1-amino-2,6-lupetidin (I), or 4-methyl-1-aminopiperazine (II), 10,11-dihydro-5H-dibenz[b,f]azepine-5-carboxylic acid chloride (III) in alc. yields the amide deriv. 10,11-dihydro-5H-dibenz[b,f]azepine-5-carboxylic acid N-(2,6-lupetidino)amide (V), or 10,11-dibenz[b,f]azepine-5-carboxylic acid N-[41-methylpiperazino]amide (VI). V and VI possess anticonvulsive, antiepileptic, and tuberculostatic activity. Thus, a mixt. of 25 g. III, 24.9 g. I and 250 ml. EtOH is heated with stirring 4 hrs. at 90.degree. and worked up to yield V, m. 131-3.degree.. VI, m. 161-3.degree. (EtOAc) is similarly prepd. from II and III.

IT **18139-42-9P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 18139-42-9 CAPLUS

CN 5H-Dibenz[b,f]azepine-5-carboxamide, N-(2,6-dimethylpiperidino)-10,11-dihydro- (8CI) (CA INDEX NAME)



L4 ANSWER 95 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:508809 CAPLUS

DOCUMENT NUMBER: 67:108809

TITLE: Cleavage of tertiary bases with phenyl chloroformate.  
 Reconversion of 21-deoxyajmaline into ajmaline

AUTHOR(S): Hobson, John Duncan; McCluskey, J. G.

CORPORATE SOURCE: Univ. Edgbaston, Birmingham, Engl.

SOURCE: J. Chem. Soc. C (1967), (20), 2015-17  
 CODEN: JSOOAX

DOCUMENT TYPE: Journal

LANGUAGE: English

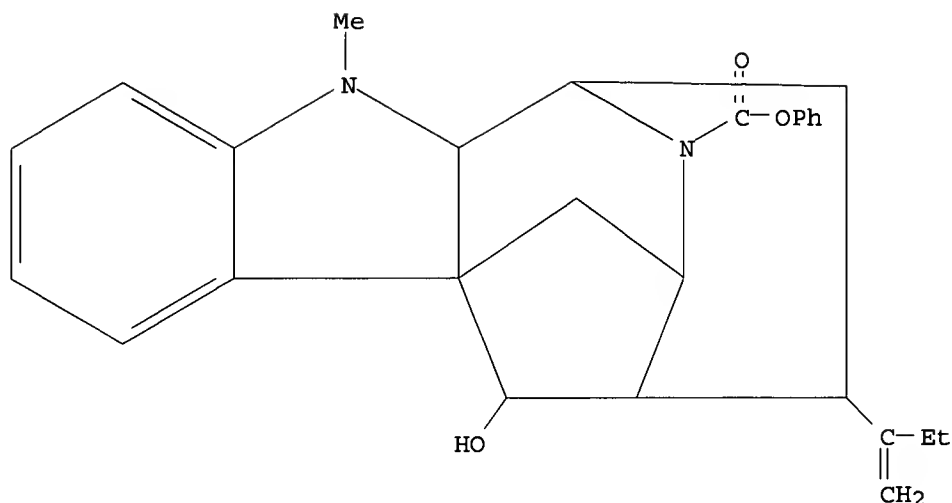
GI For diagram(s), see printed CA Issue.

AB An efficient general procedure for the cleavage of tertiary amines, involving their reaction with phenyl chloroformate under mild conditions, gives the corresponding phenyl N-carboxylates in high yield. Cleavage of 21-deoxyajmaline (I) with this reagent in the presence of LiI affords phenyl 21-iododihydrochanoajmaline-N(b)-carboxylate, which was further converted into ajmaline, thus completing a partial synthesis of ajmaline from deoxyajmalal-A.

IT **16641-69-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 16641-69-3 CAPLUS

CN 4,21-Secoajmaline-4-carboxylic acid, 21-deoxy-20,21-didehydro-, phenyl ester (8CI) (CA INDEX NAME)



L4 ANSWER 96 OF 96 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:443781 CAPLUS

DOCUMENT NUMBER: 67:43781

TITLE: Preparation and properties of 13,14-Diazatricyclo[6.4.1.12,7]tetradeca-3,5,9,11-tetraene and its derivatives

AUTHOR(S): Johnson, Alexander Lawrence; Simmons, Howard E.

CORPORATE SOURCE: E. I. du Pont de Nemours and Co., Wilmington, Del., USA

SOURCE: J. Am. Chem. Soc. (1967), 89(13), 3191-9

CODEN: JACSAT

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

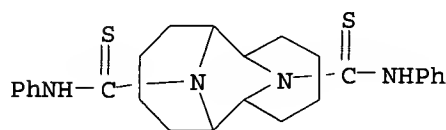
AB The thermodynamically more stable dimers of 1-cyano-, 1-ethoxycarbonyl, 1-tert-butoxycarbonyl, and 1-methylazepine are all representatives of the new 13,14-diazatricyclo[6.4.1.12,7]tetradeca-3,5,9,11-tetraene (I) ring system. These compds. are formed from kinetically produced isomers which rearrange on further thermal treatment to the doubly bridged piperazine system. The chemistry of this system and the fully reduced 13,14-diazatricyclo[6.4.1.12,7]tetradecane system is discussed in detail. 31 references.

IT 6591-86-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 6591-86-2 CAPLUS

CN 13,14-Diazatricyclo[6.4.1.12,7]tetradecane-13,14-dicarboxanilide, dithio-(8CI) (CA INDEX NAME)



=> d his



09/ 995,324

(FILE 'HOME' ENTERED AT 14:47:32 ON 09 MAY 2002)

FILE 'REGISTRY' ENTERED AT 14:47:41 ON 09 MAY 2002

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 285 S L1 FUL

FILE 'CAPLUS' ENTERED AT 14:48:37 ON 09 MAY 2002

L4 96 S L3

L5 0 S (CYCLOPENT? AND AZULEN?) AND L4

L6 0 S L4 AND AZULEN?

L7 0 S L4 AND (DITHIA AND AZA)

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

433.05

573.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-59.47

-59.47

STN INTERNATIONAL LOGOFF AT 14:53:43 ON 09 MAY 2002